

# American Crystallographic Association Annual Meeting July 25 - 29, Philadelphia, PA

**Program Chairs:**  
Louise Dawe, Kraig Wheeler

**Poster Chair:**  
Ilia Guzei

**Meeting Logo Design:**  
Jason I. Mercer

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## SATURDAY, JULY 25

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### **WK.02 Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials**

**Organizers:** Nadia Zatsepin, Edward Snell, Thomas Grant, Cornelius Gati

**Salon 3/4**

*Funding for this workshop provided, in part, by BIOXFEL, and SLAC National Accelerator Laboratory*

Serial femtosecond crystallography has yielded several major and unique advances in structural biology previously unattainable with conventional technologies, including the potential for sub-picosecond time-resolved crystallographic studies, probing cyclic or even non-cyclic reactions. With the construction of more than a dozen new XFELs currently under way, and the multiple recent demonstrations of SFX at synchrotrons, the potential user base is growing significantly. The development and appropriate use of new software to tackle the unique problems of SFX data analysis is vital to making SFX practicable.

The workshop will start with an introductory seminar, followed by most of the day dedicated to detailed hands-on tutorials with data sets collected at LCLS using the software suites Cheetah and CrystFEL, two of the most commonly used packages for SFX analysis. The concepts unique to SFX that we will be discussing are software independent.

### **WK.03 Rietveld Refinement Analysis**

**Organizers:** Clarina Dela Cruz, Oliver Gourdon

**Salon 5/6**

This all-day workshop will introduce to the attendees the use to the Rietveld analysis technique. We will first emphasize the powder diffraction technique as well as the law and rules associated with it then move on to the Rietveld quantitative technique (solution and refinement of crystallographic data). Attendees will be asked to bring their own laptops with the software already downloaded. The workshop will be primarily targeted for novice users with limited experience in diffraction want to gain expertise in using the Rietveld analysis technique.

The Rietveld method is recognized as being at the forefront of the powder diffraction refinement technique. It is of extreme importance that more people are getting expertise into this technique to have a better understanding of their technological materials of interest.

**WK.04 Small Angle Scattering:  
Structural Biology and Soft Matter****Organizer: Richard Gillian****Philadelphia North and South**

*Funding for this workshop provided, in part, by Anton Paar, DECTRIS, XENOCSS and Rigaku/Oxford Diffraction*

Small angle x-ray solution scattering (SAXS) continues to experience dramatic growth within both the structural biology and soft matter communities. While there tends to be relatively little interaction between these communities historically, the two share essentially the same basic theoretical foundation as well as a number of tools and techniques. This workshop will bring together leading SAS experts in both areas to prepare students for successful experiments.

The morning portion of the dual-track/two-room workshop will be a joint session covering theory and practice common to both fields. After the joint session, the rooms will be divided and the two parallel sessions will cover specifics of the individual fields of soft matter and structural biology. In addition to synchrotron sources, this workshop is expected to have some content devoted to laboratory x-rays sources, but also particularly neutron sources and techniques. The workshop format will

include lectures, and a selection of hands-on practical exercises. Students will be expected to bring laptops with appropriate pre-installed software as necessary. Prior to the workshop, a website (prepared by Cornell) will be configured containing installation instructions and software for each tutorial. Throughout the workshop, the emphasis will be on knowing how to judge data quality, what to do about problematic samples, and basic requirements for acceptable publication of first-time data. Students will also learn tips and tricks for home laboratory data collection and be introduced to the various national synchrotron BioSAXS beamlines and neutron sources. This workshop will also aim to educate students about the particular advantages of neutron scattering and the extra steps necessary to carry out a first SANS experiment. Selected advanced modeling techniques will also be covered.

**Saturday Evening Activities****First Time Attendee and  
Student Meeting Orientation****05:30-06:30pm Salon 10**

The focus of this informal session is to orient 'young scientists' and first time attendees to the structure of the ACA Meeting and how to make the most of their experience.

**Opening Reception Exhibit Show****07:30pm Liberty Ballroom**

Must have meeting name badge for entry

Registration Desk .....	07:30am .....	Liberty Ballroom Foyer
Speaker Ready Room .....	07:30am .....	Salon 8
Council Meeting Room.....	07:30am .....	Salon 5/6
Exhibit Show .....	10:00am .....	Liberty Ballroom
Rigaku Lunch & Learn .....	11:30am .....	Horizon's Rooftop Ballroom
Reception for Undergraduate Students.....	12:00pm.....	Philadelphia South

## P1 Warren Award Presentation & Lecture

Chris Cahill, Presiding Freedom Ballroom

08:00-08:45AM P1.01

**Understanding Oxide Surfaces: From Structure to Catalysis.** Laurence Marks.

## TR Transactions I: Crystallography for Sustainability

Cora Lind-Kovacs, Robin Rogers, Presiding

Independence AB

*Funding for this session provided, in part, by Crystal Growth & Design, Univ. of Toledo School of Green Chemistry & Engineering*

08:10-08:50AM T1.01

Metal-Organic Frameworks from Design Strategies to Applications. Mohamed Eddaudi.

08:50-09:30AM T1.02

Organic Synthesis in the Solid State Using Principles of Crystal Engineering. Leonard R. MacGillivray.

09:30-10:00AM T1.03

Crystallography and Sustainability. John R. Helliwell.

10:00-10:30AM **Coffee Break**

10:30-11:10AM T1.04

The Solvent-free Research Laboratory: Synthesis and Reaction Discovery Using Solid-state Chemistry and Mechanochemistry. Tomislav Friscic.

11:10-11:50AM T1.05

Two Step Reduction Process for the Synthesis of New Organic/Inorganic Hybrid Materials Containing Metals in Reduced Oxidation States. Hans-Conrad zur Loye.

11:50AM-01:35PM **Lunch Break**

01:35-02:15PM T1.06

Following the 'Light Atoms' in Energy Storage Devices Using Neutron Powder Diffraction. Ashfia Huq.

02:15-02:55PM T1.07

Development of Powder Diffraction Methods for Studying Complex Structural Problems in Simple Semiconductors for Solar Water Splitting. Peter Khalifah.

03:30-04:10PM T1.08

Modifications of Mo<sub>3</sub>Sb<sub>7</sub> via Chemical Substitution to Enhance the Thermoelectric Properties. Holger Kleinke.

04:10-04:50PM T1.09

Elucidating the Structure of Ionic Liquids by SXRD, SAXS and WAXS New Opportunities for Materials Design. Anja V. Mudring.

## 1.1.1 Crystallography of Emergent Phenomena I

Tyrel McQueen Jared Allred, Presiding  
Philadelphia North

09:00-09:30AM 1.1.1.01

Vacancies, Doping, and Intercalations in Solution-Produced FeSe-based Material. Kirill Kovnir, Kathleen Lee, Chongin Pak, Saeed Kamali, Joshua Greenfield.

09:30-10:00AM 1.1.1.02

White-light Emission from Layered Hybrid Perovskites. Hemamala Karunadasa, Adam Jaffe, Emma Dohner.

10:00-10:30AM **Coffee Break**

10:30-10:50AM 1.1.1.03

Structure Distortions and Spin-lattice Coupling in EuTiO<sub>3</sub>. HuiBo Cao, Jiaqiang Yan, Bryan C. Chakoumakos.

Canadian Division Meeting .....	12:00pm .....	Independence AB
Industrial SIG Meeting .....	12:00pm .....	Independence CD
General Interest Meeting.....	05:00pm .....	Freedom
Poster Session S (sponsored by Art Robbins).....	05:30pm .....	Liberty Ballroom
Bruker YSSIG Mixer (ticket required).....	08:00pm .....	City Tap House-Logan Square

**10:50-11:10AM** **1.1.1.04**  
 Observation of the Magnetic C4 Phase and a Two Q Magnetic Structure in Hole Doped  $Sr_{1-x}Na_xFe_2As_2$ . Keith M. Taddei, Omar Chmaissem, Saul Lapidus, Mercouri G. Kanatzidis, Duck Young Chung, Helmut Claus, Dennis Brown, Raymond Osbron, Stephan Rosenkranz, Matthew Krogstad, Daniel Bugaris, Jared Allred.

**11:10-11:40AM** **1.1.1.05**  
 Magnetic Ordering and Metal-insulator Transitions in Hollandite-type Oxides. Efrain E. Rodriguez, Pouya Moetakef, Amber Larson.

**11:40-12:00PM** **1.1.1.06**  
 Syntheses, Crystal Structure and Properties of  $Ca_3RE MnSb_{11}$  (RE = La-Sm). New Quaternary Phases Derived from  $Ca_{14}MnSb_{11}$ . Jai Prakash, Svilen Bobev.

**1.1.2 Poster Preview**  
**Louise Dawe, Bill Duax, Presiding**  
**Philadelphia South**

**9:00-9:10AM** **M25**  
 Synthesis and Characterization of a Bismuth (III)-Organic Hybrid Material. Alyssa K. Adcock, Karah E. Knope.

**9:10-9:20AM** **M39**  
 Novel Uranyl(VI) Complexes Incorporating Propylene-bridged Salen-type  $N_2O_2$ -ligands: A Structural Approach. Saud I. Al-Resayes, Mohammad Azam.

**9:20-9:30AM**

**9:30-9:40AM** **T46**  
 Structure-guided Modification of a Flavin-Dependent Isoprenoid Alkene Reductase. Yan Kung, Jay D. Keasling, Paul Adams, Jose H. Pereira, Charlie C. Liu, Xinkai Xie, Ryan P. McAndrew.

**9:40-9:50AM** **M13**  
 Study of the Natural Growth Desert Rose Formations, in Particular from the Desert of Chihuahua, a Structural and Chemical Behavior Analysis. Andres Jose Encerrado Manriquez, Alex D. Price.

**9:50-10:00AM**

**10:00-10:30AM** **Coffee Break**

**10:30-10:40AM** **S11**  
 Crystal Structure of a Drug Target Midazole-glycerol-phosphate Dehydratase (IGPD) from *Mycobacterium tuberculosis*. Mohd S. Ahangar.

**10:40-10:50AM** **T17**  
 Earliest Robosomal Proteins Had No Methionine to Begin With. William Duax, Nick Sass, Connor Huck, Sam Chen.

**10:50-11:00AM** **T02**  
 A Novel Cyclization Mechanism to Biologically Produce Pharmacological Cyclic Compounds: The Crystal Structure of a Terpenoid Cyclase Derived from Short Chains Dehydrogenase/Reductases. Sheng Ye, Rongguang Zhang, Yun Zhu, Lili Qin.

**11:00-11:10AM** **S16**  
 Effect of Environmental Pollutants on Xenobiotic Regulation via P-glycoprotein (P-gp). Steven Rees, Geoffrey Chang, Aaron P. McGrath.

**11:10-11:20AM** **S04**  
 Beclin 2 Interacts with Atg14 Through a Metastable Coiled-coil to Regulate Autophagy. Minfei Su, Sangita Sinha, Christopher L. Colbert, David Neau, Yue Li.

**11:20-11:30AM**

**11:30-11:40AM** **S36**

Structural and Functional Characterizations of Solute Binding Proteins by Differential Scanning Fluorimetry and Crystallography. Umesh Yadava, Steven C. Almo, J.A. Gerlt, K.L. Whalen, R.D. Siedel, J. Love, Rafael Toro, N.F. Al Obaidi, Matthew W. Vetting.

**11:40-11:50AM** **T14**

DISTRO\_PDB: Probing Crystallographic Data Distributions and Correlations in the Protein Data Bank. Huanwang Yang, Stephen K. Burley, Helen M. Berman, John D. Westbrook, Jasmine Young, Chenghua Shao, Brian P. Hudson.

**11:50-12:00PM** **S10**

Crystal Structure and Receptor Binding of the Haemagglutinin from Human-infecting H10N8 Influenza Virus. Heng Zhang, Ian A. Wilson, James Paulson, Ryan McBride, Wenli Yu, Xueyong Zhu, Netanel Tzarum, Robert de Vries.

## **1.1.3 Application of SANS/SAXS to Structural Biology**

**Kushol Gupta Alvin Acerbo, Presiding**  
**Freedom Ballroom**

**09:00-09:20AM** **1.1.3.01**

Applications of Small-Angle Neutron Scattering to Membrane Structural Biology. William Heller.

**09:20-09:40AM** **1.1.3.02**

Order-to-Disorder Transitions in BECN1 Regulate Autophagy. Sangita Sinha, Christopher L. Colbert, Srinivas Chakravarthy, Ruslan Sanishvili, Arvind Ramanathan, Minfei Su, Karen Glover, Yang Mei.

**09:40-10:00AM** **1.1.3.03**

Shape of the CENP-A Nucleosomes in Solution on  $\alpha$ -satellite DNA is Different than on Synthetic "601" DNA Sequence. Nikolina Sekulic, Ben Black, Greg Van Duyne, Kuhol Gupta.

**10:00-10:30AM Coffee Break**

**10:30-10:50AM** **1.1.3.04**

Small-Angle X-ray and Neutron Scattering Studies of HIV-1 Proteins and their Interactions. Jill Trehwella.

**10:50-11:10AM** **1.1.3.05**

Serial SAXS and Crystallization *in-situ*: New Options for Automated, Efficient and High Throughput Data Acquisition at the ESRF Biosaxs Beamline BM29. Adam R. Round, Sebastien Teychené, Françoise Bonneté, Beatrice Biscans, Nhat Pham, Dmitri Radajewski, Martha Brennich, Petra Pernot.

**11:10-11:30AM** **1.1.3.06**

SANS Contrast Variation Experiments on Protein Complexes with Disordered Subunits. Susan Krueger.

**11:30-11:50AM** **1.1.3.07**

CCP-SAS A Community Consortium for the Atomistic Modelling of Scattering Data. Joseph E. Curtis, Stephen Perkins, Paul Butler, Stephen King, Jianhan Chen, Hailiang Zhang, David W. Wright, Emre Brookes.

## **1.1.4 Structural Informatics for Drug Design and Development**

**Mark Oliveira, Presiding**  
**Independence AB**

**09:00-09:30AM** **1.1.4.01**

Exploring Structure-stability Relationships of Tazofelone Polymorphs. Susan Reutzle-Edens.

**09:30-10:00AM** **1.1.4.02**

Identifying Intermolecular Interactions that Influence Crystal Packing and Symmetry. Robin Taylor, Jason Cole, Frank Allen.

**10:00-10:30AM Coffee Break**

**10:30-11:00AM** **1.1.4.03**

A Comprehensive Database of Distance Geometry Enables Rapid Searches for Likeness in PDB Structures and Complexes. Barry C. Finzel.

**Undergraduate Reception**

**Sponsored by the Society of Physics Students  
Philadelphia South 12:00 - 01:30pm**



All students, mentors, as well as others who might be interested, are invited to join us for a reception highlighting undergraduate research. Posters by undergraduates will be presented in this special undergraduate-focused session. In addition, Dr. William Duax, ACA CEO, Hauptman-Woodward Institute, will give a talk entitled "Harker, Hauptman, Hodgkin and Me." Refreshments will be provided.

**11:00-11:20AM**

**1.1.4.04**

Rational Engineering of Protein Surfaces to Improve Crystallization While Preserving Solubility. Shikha Singh, John Hunt, Gaetano Montelione, Rong Xiao, Thomas Acton, John Everett, Min Su, Samuel Handelman, Alexandre Kuzin, Farhad Forouhar, Sergey Vorobiev, Helen Neely, W. Nicholson Price, Victor Naumov.

**11:20-11:40AM**

**1.1.4.05**

Using Small Molecule Structures to Generate High Quality Dictionaries for Macromolecular Refinement of Protein-Ligand Complexes. Paul Emsley.

**11:40-12:00PM**

**1.1.4.06**

Including Cis-peptides in a Conformation Dependent Library for Protein Main Chain Bond Angles. Dale E. Tronrud, P. A. Karplus.

**1.2.1 From Fingerprinting to Full ID: PXRD**

**Curt Haltiwanger, Richard Staples, Presiding  
Philadelphia North**

*Funding for this session provided, in part, by Panalytical, Bruker and Rigaku/Oxford Diffraction*

**01:30-02:00PM**

**1.2.1.01**

Applications of Powder X-ray Diffraction in Pharmaceutical Development. Andrew P. Brunskill.

**02:00-02:30PM**

**1.2.1.02**

Quantitative Analysis by X-ray Powder Diffraction: Chemometrics, Matrix Effects and Non-crystalline Materials. Simon Bates.

**02:30-03:00PM**

**1.2.1.03**

Pair Distribution Function using Laboratory X-Ray Diffraction Equipment. Julie E. Quinn, Milen Gateshki, Celeste A. Reiss, Marco Sommariva.

**03:00-03:30PM Coffee Break**

**03:30-04:00PM**

**1.2.1.04**

Non Classical Applications of Powder Diffraction and the Rietveld Method: From Thin Films, Nanomaterials to Texture and Residual Stress Analyses. Luca Lutterotti.

**04:00-04:30PM**

**1.2.1.05**

Pharmaceutical Materials Science Unique Role of XRD in the Characterization and Quantification of Crystalline Phases. Raj Suryanarayanan.

**04:30-05:00PM**

**1.2.1.06**

XRD2 and XRD3 Analyses of Polycrystalline Powders, Solids and Films. Jim Britten, Vicky Jarvis.

**1.2.2 Engaging Undergraduates with Crystallographic Research**

**Roger Rowlett, Joe Tanski, Presiding  
Freedom Ballroom**

*Funding for this session provided, in part, by Art Robbins Instruments*

**01:30-02:00PM**

**1.2.2.01**

X-Ray Diffraction in Forensic Chemistry Curriculum: Some Remarks from State College Laboratory. Alexander Y. Nazarenko.

**02:00-02:30PM**

**1.2.2.02**

Assessing the Structural Effects of Unnatural Amino Acid Incorporation in Proteins; Setting up and Maintaining a Protein X-Ray Crystallography Lab at a Small Liberal Arts College. Christine M. Phillips-Piro.

**02:30-03:00PM**

**1.2.2.03**

One Crystal Structure a Day. James A. Golen, David R. Manke.

## 03:00-03:30PM Coffee Break

### 03:30-04:00PM 1.2.2.04

Using Crystallography to Lower the Barriers to Starting Research with Undergraduates. Dean H. Johnston.

### 04:00-04:30PM 1.2.2.05

X-ray Crystallography as a Central Technique in Undergraduate Research. Paul D. Cook.

### 04:30-05:00PM 1.2.2.06

Asymmetric Carbonyl and Imine Alkylation With Titanium Lewis Acid Catalysts: Ligands, Metal Complexes, Substrates and Products, Incorporating Chemical Crystallography All the Way. Joseph Tanski.

## 1.2.3 Molecular Machines

**Tim Maier, Presiding**  
**Philadelphia South**

*Funding for this session provided, in part, by Molecular Dimensions*

### 01:30-02:10PM 1.2.3.01

A Hybrid Methods Approach to Determine the Structure of *Tetrahymena* telomerase holoenzyme. Juli Feigon.

### 02:10-02:35PM 1.2.3.02

Bacterial Microcompartments: Selective Molecular Transport through Shell Pores. Sunny Chun, Todd Yeates, Thomas Bobik, Sharmistha Sinha, Michael Sawaya, Allan Pang, Chiranjit Chowdhury, Daegwin Jeong.

### 02:35-03:00PM 1.2.3.03

Structural Studies on the Yeast and Human U6 snRNPs. Eric J. Montemayor, Samuel E. Butcher, David Brow.

## 03:00-03:30PM Coffee Break

### 03:30-04:10PM 1.2.3.04

Crystal Structure of the Polycomb PRC1 E2-E3 Ubiquitylation Module Bound to its Nucleosome Substrate. Song Tan, Ryan C. Henrici, Robert K. McGinty.

### 04:10-04:35PM 1.2.3.05

Atomic Insights into the Protein Phosphatase-1 Holoenzymes. Rakhi Bajaj, Rebecca Page, Peti Wolfgang.

### 04:35-05:00PM 1.2.3.06

A Pyruvate Dehydrogenase-Dihydrolipoyl Acetyltransferase Subcomplex from the Pyruvate Dehydrogenase Multi-enzyme Complex Reveals Lipoyl Domain-E1 Interactions and a Novel Tethering Mode Linking the E1 and E2 Components. William Furey, Frank Jordan, Natalia Nemeria, Guillermo A. Calero, Shelley Reynolds, Palaniappa Arjunan.

## 1.2.4 Biological Macromolecules

**Ed Collins, Andy Howard, Presiding**  
**Independence CD**

### 01:30-01:50PM 1.2.4.01

RitR, A Response Regulator with an Aspartate-Less Receiver Domain. Lanlan Han.

### 01:50-02:10PM 1.2.4.02

Structural Insight into the Deubiquitinating Activity of MERS-CoV PLpro Demonstrates its Role in the Suppression of the Innate Immune Response. Ben A. Bailey-Elkin, Brian L. Mark, Marjolein Kikkert, Eric J. Snijder.

### 02:10-02:30PM 1.2.4.03

Structural and Biochemical Characterization of *Pseudomonas putida* KT2440 NicC, a 6-Hydroxynicotinic Acid 3-Monooxygenase. Katherine Hicks, Mark Snider, Tyler Gerwig, Megan Kopp, Weifeng Zhen, Meigan Yuen.

### 02:35-02:55PM 1.2.4.04

Cyclic-di-AMP Promotes Bacterial Virulence Through Allosteric Regulation of Pyruvate Carboxylase. Philip Choi, Liang Tong, Joshua Woodward, Kamakshi Sureka.

## 02:55-03:30PM Coffee Break

### 03:30-03:50PM 1.2.4.05

Early Structure Based Design on the way to Novel Binding of ERK Inhibitors. Alan Hruza.



**03:55-04:15PM**

**1.2.4.06**

A Life-Science and Biomedical Technology Research Resource for NSLS-II LSBR. Robert M. Sweet, L. Yang, R. Tappero, V. Stojanoff, D. K. Schneider, A Soares, J. M. Skinner, H. Robinson, A. M. Orville, L. Miller, S. McSweeney, J. Jakoncic, A. Heroux, M. R. Fuchs, S. Chodankar, L. E. Berman, S. Kim, K. H. Kim, M. S. Chung, C. Lee, A. E. Cho, K. R. Han, J.-H. Lee, G. Gowda, D. B. Lee, Y. B. Chung, J. H. Seok, S. W. Jung, Y.-H. Park.

**04:15-04:35PM**

**1.2.4.07**

Innovative Applications of Pressure Cryocooling. Teck Khiang Chua, Marian Szebenyi, Qingqiu Huang.

**04:40-05:00PM**

**1.2.4.08**

MX Structural Solution using ccp4 and ccp4i2. Charles Ballard, Gwyndaf Evans, Marcin Wodjyr, Ville Uski, David Waterman, Andrey Lebedev, Ronan Keegan, Eugene Krissinel, Stuart McNicholas, Kevin Cowtan, Liz Potterton, Martin Noble.

**1.3.1 Career Odyssey**

**George Lountos, Presiding**  
**Philadelphia South**

**05:00-06:30PM**

This session will feature the following panelists from the crystallographic community within diverse career tracks. It will be an interactive session in which the speakers will share how they decided to pursue their current career path, what their jobs entail and useful tips for career transition. The platform will then open for discussion and questions from the audience.

*Panelists:*

Celeste MacElver  
Pharmacokineticist, Nuventra Inc.

Christine Beavers  
COMPRES/Advanced Light Source

Cora Lind-Kovacs  
University of Toledo

Jason Stagno  
NCI, NIH

Steven Sheriff  
Bristol Myers Squibb R&D

**BRUKER Young Scientists SIG Mixer**

High energy fun, great food and some of the most exciting venues make the Young Scientists Mixer a great place to connect with scientists ranging in experience and disciplines. The Sunday night mixer is one of the meeting's most popular events and is **FREE** to registered Students & Postdocs (**ticket required; pick one up at the Registration Desk**) and \$30 for all others. The mixer will be held at City Tap House Logan, 2 Logan Square, Philadelphia, [www.citytaphouselogan.com](http://www.citytaphouselogan.com). Mixer begins at 8:00pm. This event is sponsored in part, by Bruker, AXS.



# MONDAY, JULY 27

Registration Desk .....	7:30am .....	Liberty Ballroom Foyer
Speaker Ready Room .....	7:30am .....	Salon 8
Council Meeting Room.....	7:30am .....	Salon 5/6
Exhibit Show .....	10:00am.....	Liberty Ballroom
Young Scientists SIG Meeting .....	12:00pm .....	Independence AB

## P2 Buerger Award Presentation & Lecture

Chris Cahill, Presiding

Freedom Ballroom

08:00-08:45AM

Gregory Petsko

### 2.1.1 Porous Materials at the Nano and Meso-scale

Craig Brown, Presiding

Philadelphia North

*Funding for this session provided, in part, by Royal Society of Chemistry*

**09:00-09:40AM** **2.1.1.01**

Symmetry and Electronic Structure Considerations in the Synthesis of Electrically Conducting MOFs. Mircea Dinca.

**09:40-10:00AM** **2.1.1.02**

*In-situ* Powder Diffraction of Small Molecules in Industrially Relevant Porous Materials. Matthew Hudson, Craig Brown.

**10:00-10:30AM** **Coffee Break**

**10:30-11:00AM** **2.1.1.03**

Metal-organic Frameworks, Hydrogen Bonded Organic Frameworks, and Jesse Rowsell. Stephen FitzGerald, Orhan Talu, Charles F. Campana, Matthias Zeller, Josh Greenfield, Ren Wiscons, Holden Lai, Cassandra Zentner.

**11:00-11:20AM** **2.1.1.04**

*In-situ* Powder Diffraction Studies of High-Pressure Gas Loading in Metal-Organic Frameworks. Andrey A. Yakovenko, Gregory Halder.

**11:20-11:40AM** **2.1.1.05**

Ultrasmall Angle X-ray Scattering (USAXS) and Wide-Angle X-ray Scattering (WAXS) Studies on the Complex Metal Hydride  $\text{NaAlH}_4$ . Tabbetha Dobbins, James Torres, Christopher Bennett, Jan Ilavsky.

### 2.1.2 Crystal Engineering Form & Function

Peter Wood, Tomislav Friščić, Presiding

Philadelphia South

**09:00-09:30AM** **2.1.2.01**

Explosive Cocrystals. Adam J. Matzger.

**09:30-10:00AM** **2.1.2.02**

Semiconductor Co-Crystals. Leonard R. MacGillivray.

**10:00-10:30AM** **Coffee Break**

**10:30-11:00AM** **2.1.2.03**

MOFs as Macromolecular Ligands: New Coordination Chemistry Enabled by SBU Transmetalation. Mircea Dinca.

**11:00-11:20AM** **2.1.2.04**

Programmable Crystal Contacts Used to Improve the Resolution of Self-Assembled 3D DNA Crystals. Nadrian C. Seeman, Yoel Ohayon, Arun R. Chandrasekaran, Carina Hernandez, Jens J. Birktoft, Ruojie Sha, Philip Lukeman, Chengde Mao, Paul Chaikin, Stephan Gine.

**11:20-11:40AM** **2.1.2.05**

Melting Point-solubility-structure Relations of Selected Inclusion Compounds. Nikoletta Bathori.

**11:40-12:00PM** **2.1.2.06**

The Role of Atropisomers on the Photo-reactivity and Fatigue of Diarylethene-based Metal-organic Frameworks. Jason B. Benedict, Yu-Sheng Chen, Dinesh G. Patel, Cassidy Benson, Cody Gleason, Jordan Cox, Ian Walton.

Materials/Neutron/Powder SIG Joint Meeting .....	12:00pm .....	Philadelphai North
Fiber Diffraction SIG Meeting.....	12:00pm .....	Philadelphia South
Meet-the-Editors, IUCr Journals .....	03:00pm .....	IUCR Booth 302
Light Sources SIG Meeting.....	05:00pm .....	Independence AB
Poster Session M.....	05:30pm .....	Liberty Ballroom

**2.1.3 General Interest**

**Stacey Smith, Presiding**  
**Independence CD**

**09:00-09:30AM** **2.1.3.01**  
Reaching a New Highpoint with Crystallography Software - APEX3. Michael Ruf, Bruce C. Noll Joerg Kaercher.

**09:30-10:00AM** **2.1.3.02**  
Upgrading Experimental Setups with Incoatec's Microfocus Source I  $\mu$ S and/or Scatterless Pinholes. Andreas Kleine, Jorgen Graf, Lars Kuttnik, Christopher Umland.

**10:00-10:30AM** **Coffee Break**

**10:30-11:00AM** **2.1.3.03**  
Current Status of the Liquid-Metal-Jet X-ray Source Technology. Emil Espes, Goran Johansson, Per Takman, Oscar Hemberg, Bjorn A. Hansson, Tomi Tuohimaa, Mikael Otendal.

**11:00-11:20AM** **2.1.3.04**  
The Routine use of D8 VENTURE with MET-ALJET Systems in Chemical Crystallography and Structural Biology Laboratories. Charles F. Campana, Severine Freisz, Matthew Benning, Bruce C. Noll.

**11:20-11:40AM** **2.1.3.05**  
Extracting an Extremely Weak Sulfur SAD Signal using Shutterless Data Collection and a High-Speed CCD Detector. Zheng-Qing Fu, Bi-Cheng Wang, John P. Rose, John Gocny, Rod Salazar, James Fait, Unmesh Chinte, Palani Kandavelu, Zhongmin Jin, John Chrzas.

**11:40-12:00PM** **2.1.3.06**  
What's New in GSAS-II. Brian Toby, Robert Von Dreele.

**2.1.4 Publication Practices**

**Larry Falvello, Presiding**  
**Independence AB**

*Funding for this session provided, in part, by Crystallographic Resources*

**09:00-09:30AM** **2.1.4.01**  
Publication of a Thousand Structures a Day. Suzanna C. Ward, Peter A. Wood, Colin R. Groom.

**09:30-10:00AM** **2.1.4.02**  
On the Proper Reporting and Archival of Crystal Structure Data. Anthony Spek.

**10:00-10:30AM** **Coffee Break**

**10:30-11:00AM** **2.1.4.03**  
Crystallography from all Sides. Phillip E. Fanwick.

**11:00-11:30AM** **2.1.4.04**  
The Role of IUCr Journals in the Chemical Space. Alexander J. Blake.

**2.1.5 Structural Dynamics**

**George Phillips, Presiding**  
**Freedom Ballroom**

*Funding for this session provided, in part, by American Institute of Physics Publishing*

**09:00-09:30AM** **2.1.5.01**  
Time-Resolved (Serial) Crystallography at the Synchrotron and at the X-ray FEL. Marius Schmidt.

**09:30-10:00AM** **2.1.5.02**  
Time Resolved Studies of Molecular Triplet States. Scaling of Multi-crystal Data Sets and Results. Philip Coppens, Bertrand Fournier.

**10:00-10:30AM** **Coffee Break**

**10:30-10:45AM** **2.1.5.03**  
Studies of Enzyme and Photoreceptor Dynamics. George N. Phillips Jr., Mitchell D. Miller,

# MONDAY, JULY 27

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Jose L. Olmos Jr., Jonathan A. Clinger.

**10:45-11:00AM** **2.1.5.04**

Fourier-transform Inelastic X-ray Scattering using Free Electron Laser Pulses. Mariano Trigo, David Reis, Diling Zhu.

**11:00-11:15AM** **2.1.5.05**

Flexibility and Structural Studies of Antibodies with Crosslinked Antigens. D.T. Gallagher, Ioannis Karageorgos.

**11:15-11:30AM** **2.1.5.06**

Ligand Substitution and Guest Exchange in a Metal-Organic Framework Monitored by *in situ* X-ray Diffraction Techniques. Jordan Cox, Jason B. Benedict, Yu-Sheng Chen, Travis Mitchell, Gage Bateman, Eric Sylvester, Cassidy Benson, Ian Walton.

**11:30-11:55AM** **2.1.5.07**

Frontiers in Conformational Mapping of Molecular Machines in Biology. Ali Dashti, Abbas Ourmazd, Joachim Frank, Wen Li, Hstau Liao, Russell Fung, Ahmad Hosseinizadeh, Peter Schwander.

## **2.2.1 Advances in Multi-crystal Approaches & Serial Crystallography**

**Nadia Zatsepin, Presiding**  
**Independence AB**

**01:30-02:00PM** **2.2.1.01**

What's Different About XFEL Crystallography? John C. Spence.

**02:00-02:30PM** **2.2.1.02**

Using all Your Data in Spite of Non-isomorphism. James Holton, Marius Schmidt.

**02:30-03:00PM** **2.2.1.03**

Recovering Protein Crystal Orientation from Nindexable Data Frames. Jennifer Wierman, Ti-Yen Lan, Mark Tate, Hugh Philipp, Veit Elser, Sol Grun.

**3:00-3:30PM Coffee Break**

**03:30-04:00PM** **2.2.1.04**

Serial Crystallography on Beamline P14@PETRAIII. Gleb P. Bourenkov, Thomas R. Schneider, Ivars Karpics.

**04:00-04:30PM** **2.2.1.05**

Multicrystal Data Collection and Analysis at Diamond Light Source. Danny Axford, Gwyn-daf Evans, Graeme Winter, Robin L. Owen, Jose Trincao, James Foadi, Richard Gildea, Anna Warren.

**04:30-05:00PM** **2.2.1.06**

Lower-Energy Native-SAD Phasing from Multiple Crystals. Qun Liu, Wayne Hendrickson.

## **2.2.2 Materials Discovery and Crystal Growth**

**Paul Forster, Efrain Rodriguez, Presiding**  
**Independence CD**

**01:30-02:00PM** **2.2.2.01**

Octahedral Tilting and Cation Ordering in Layered Perovskites. Patrick M. Woodward, Ryan Morrow, Andrew Sharits.

**02:00-02:20PM** **2.2.2.02**

A New Family of Compounds with Distorted Diamond-like Structures. Jennifer A. Aitken, Kimberly A. Rosmus, Jian-Han Zhang, Jacilynn A. Brant, Charles W. Sinagra.

**02:20-02:40PM** **2.2.2.03**

Syntheses, Crystal Chemistry and Electronic Properties of  $A_{14}Cd_{1+x}Pn_{11}$  Compounds ( $0 \leq x \leq 0.27(1)$ ; A = Sr, Eu; Pn = As, Sb): Non-stoichiometric Compositions Arising from Synergistic Electronic and Size Effects. Julien Pierre Amelie Makongo Mangan, Svilen Bobev.

**02:40-03:00PM** **2.2.2.04**

Defects and Magnetism in  $(BaF)_2Fe_{2-x}Q_3$  ( $Q=S, Se$ ). Jared Allred, Mercouri G. Kanatzidis, Duck Young Chung, Fei Han, Daniel E. Bugaris, Christos Malliakas, Mihai Sturza.

**3:00-3:30PM Coffee Break**

**03:30-04:00PM** **2.2.2.05**

Crystal Chemistry and Thermoelectric Properties of Ba-M-P (M= Ni, Cu, Au) Clathrates: Phase Transformations Induced by Electron Doping. Kirill Kovnir.

**04:00-04:30PM** **2.2.2.06**

Structure-property Relationships in Magnetic Intermetallics Grown from Rare Earth-rich Melts. Susan Latturmer, Huibo Cao, Sixuan Zhou.

**04:30-05:00PM** **2.2.2.07**

Group IV Graphane Analogues. Josh Goldberger, Maxx Arguilla, Shishi Jiang.

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

**Amy Sarjeant, John Lee, Presiding**  
**Freedom Ballroom**

**01:40-02:10PM** **2.2.3.01**

Crystallography at Remote Undergraduate Institutions - From Simplicity to Sophistication. Stephanie K. Hurst, Samantha Kruse.

**02:10-02:30PM** **2.2.3.02**

An Investigation of Cationic bis-cyclometalated Iridium Complexes Through X-ray Crystallography. Lauren A. Mitchell, Bradley J. Holliday, Jason D. Slinker, Yulong Shen, Lyndon D. Bastatas, Kristin J. Suhr.

**02:30-03:00PM** **2.2.4.03**

Crystal Engineering of the Metal-Metal Bond: New Developments in Material Design. Christopher Durr.

**3:00-3:30PM Coffee Break****03:30-04:00PM** **2.2.3.04**

Coming Back to Crystallography: How the ACA Summer School Helped Start a New Direction in Research and Teaching. Dean H. Johnston.

**04:00-04:20PM** **2.2.3.05**

How One Summer Vacation Created an Active Research Program for a Novice Crystallographer, Working with Undergraduate Researchers, and in Direct Possession of a Single-Crystal X-ray Diffractometer. John P. Lee.

**04:20-04:40PM** **2.2.3.06**

Mineral Crystallography: Unexpected Applications of Knowledge Gained from a Small Molecule Summer School. Nichole R. Valdez.

**2.2.4 SAS with Membranes and Membrane Proteins**

**Fred Heberle, Shuo Qian, Presiding**  
**Philadelphia North**

**01:30-02:00PM** **2.2.4.01**

Bicontinuous Microemulsions: A Valuable Biomembrane Mimetic System for Melittin. Volker S. Urban, Rachel N. Dunlap, Ran Ye, Sai Venkatesh Pingali, Hugh M. O'Neill, Douglas G. Hayes.

**02:00-02:25PM** **2.2.4.02**

Determining Micelle and Bicelle Size and Shape with Small-angle Scattering. Ryan Oliver, Linda Columbus, Jan Lipfert.

**02:25-03:00PM** **2.2.4.03**

Probing Membrane Protein Structure with Small-Angle Scattering and Molecular Modeling. Marc F. Lensink, Christine Ebel, Françoise Jacob-Dubuisson, Vincent Villeret, Bernard Clantin, Frank Gabel.

**3:00-3:30PM Coffee Break****03:30-04:05PM** **2.2.4.04**

Asymmetric liposomes: assessing lipid composition, distribution and structure. Drew Marquardt, Georg Pabst, John Katsaras, Barbara Geier, Milka Doktorova, Frederick A. Heberle.

**04:05-04:30PM** **2.2.4.05**

Water Distribution in Membrane Fusion Intermediates Revealed by Neutron Membrane Diffraction. Shuo Qian.

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## 2.2.5 Mechanistic & Spectroscopic Structural Enzymology

**Mohammad Taha, Presiding**  
Philadelphia South

*Funding for this session provided, in part, by MiTiGen*

### 01:30-02:00PM 2.2.5.01

Protein Flavinylation in Bacteria: Structural and Biochemical Insights from the Catalytic Core of Periplasmic Flavin-trafficking Protein (Ftp) and its Flavoprotein Product. Diana R. Tomchick, Michael V. Norgard, Wei Z. Liu, Chad A. Brautigam, Ranjit K. Deka.

### 02:00-02:30PM 2.2.5.02

The Role of Oxyanion Holes in the Structure and Function of Type III Polyketide Synthases. Charles Stewart, Joseph P. Noel.

### 02:30-03:00PM 2.2.5.03

Orthoester Cyclization in Orthosomycin Biosynthesis is Catalyzed by a Family of Nonheme Iron,  $\alpha$ -ketoglutarate Dependent Enzymes. Kathryn McCulloch, T. M. Iverson, Brian Bachmann, Bryan Gitschlag, Jeannette Mathieu, Emilianne McCranie.

### 3:00-3:30PM Coffee Break

### 03:30-04:00PM 2.2.5.04

Crystal Structure of a Type II Extradiol Dioxxygenase PraA. Toshiya Senda, Keisuke Sugimoto, Miki Senda.

### 04:00-04:20PM 2.2.5.05

High Resolution Crystal Structure of the Cancer-Associated Carbonic Anhydrase IX. Brian P. Mahon, Robert McKenna, Antonette Bennett, Farzaneh Tondnevis, Lilien Socorro, Jenna M. Driscoll.

### 04:20-04:40PM 2.2.5.06

Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography. Flora Meilleur.

### 04:40-05:00PM 2.2.5.07

Conservation and Functions of Carbon-Oxygen Hydrogen Bonding in AdoMet-Dependent Methyltransferases. Raymond Trievel, Hashim

Al-Hashimi, Steve Scheiner, Robert L. Houtz, Ryan A. Mehl, Paul A. Del Rizzo, Upendra Adhikari, Joseph D. Yesselman, Lynnette M. Dirk, Scott Horowitz.

## 2.3.1 Professional Development: Communicating Your Science

**Jarrold French, Andy Torelli, Presiding**  
Philadelphia South

### 05:00-05:18PM 2.3.1.01

Understanding Your Audience: Advice from American Chemical Society Science & the Congress Project and also Chemistry Champions to Help Craft Better Messages for 'the General Public'. Darcy Gentleman, American Chemical Society.

### 05:18-05:36PM 2.3.1.02

Considerations for Communicating Science in a Regulatory Forum. Celeste MacElrevey, Nuventra Pharma Sciences Inc.

### 05:36-05:54PM 2.3.1.03

Communicating Science to the Public. Amalia Issa, University of the Sciences.

### 05:54-06:12PM 2.3.1.04

Effective Communication Between the Extramural Scientific Community the NIH. Joseph Gindhart, National Institutes of Health.

### 06:12-06:30PM 2.3.1.05

Improving Impact and Clarity in your Written Communications. Katherine Sippel, BioScience Writers, LLC..

**2.3.2 Would You Publish This?**

**Louise Dawe, Brian Dolinar, Presiding  
Philadelphia North**

*Funding for this session provided, in part, by Crystallographic Resources*

**08:00-08:15PM** **2.3.2**  
Introduction to Would You Publish This? Allen Oliver.

**08:15-08:30PM** **2.3.2.01**  
The Same But Chillier - Should We Publish? Carl H. Schwalbe, Miren Ramirez.

**08:30-08:45PM** **2.3.2.02**  
Nobody Told Me There'd Be Structures Like These. Carla Slebodnick, Paul Deck, Charles Carfagna, Rachele Piemonte.

**08:45-09:00PM** **2.3.2.03**  
Built Like A MOF - But A Purely Organic Cage. Lee Daniels, Michael Mastalerz, Iris Oppel, Fraser White, Oliver Presly, Gang Zhang.

**09:00-09:15PM** **2.3.2.04**  
Crystals Undergoing Transformations: Ugly yet Useable? Hideous but Helpful? Appalling and Appealing! Christine M. Beavers, Simon J. Teat.

**09:15-09:30PM** **2.3.2.05**  
Would you Publish a Tetrahedral Pt(II) Complex with R=2.7%? Frank R. Fronczek, Svetlana Pakhomova.

**2015 Margaret C. Etter Student Lecturer Awards**

Each Scientific Interest Group (SIG) has the opportunity to select one student to receive an award and to present a lecture. Selections are based upon submitted abstracts and are independent of whether the student originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of \$250 and a certificate to be presented at the beginning of their lecture.

**CONGRATULATIONS TO THESE WINNERS:**

- BioMac..... Philip Choi, Columbia Univ..... 1.2.4.04
- General Interest ..... Pawel Janowski, Rutgers Univ..... 3.1.1.06
- Industrial ..... Brian Mahon, Univ. of Florida ..... 2.2.5.05
- Light Sources ..... Pascal Krotee, Univ. of Calif.-Los Angeles ..... 3.1.1.08
- Materials Science ..... Mariana Verezhak, Univ. of Grenoble, France .. 4.2.4.06
- Neutron Scattering... Keith Taddei, Northern Illinois Univ. .... 1.1.1.04
- Powder Diffraction ... Daniel Mast, Univ. of Nevada ..... 3.1.1.02
- Small Molecule..... Karina Heffernan, Virginia Tech ..... 4.2.2.02
- Young Scientist ..... Katarzyna Handing, Univ. of Virginia ..... 3.1.1.05

Registration Desk .....	07:30am .....	Liberty Ballroom Foyer
Council Meeting Room.....	07:30am.....	Salon 5/6
Speaker Ready Room .....	07:30am.....	Salon 8
Exhibit Show .....	10:00am.....	Liberty Ballroom
BioMac SIG Meeting.....	12:00pm.....	Freedom Ballroom

## P3 Margaret Etter Early Career Award and Lecture

Chris Cahill, Presiding Philadelphia South

08:00-08:45AM P3.01

Nature, Imitation Game: Decipher the Combinatorial CTD Code for Eukaryotic Transcription. Yan Jessie Zhang.

### 3.1.1 Etter Early Career Symposium

George Lountos, Andrey Yakovenko, Presiding Philadelphia South

09:00-09:20AM 3.1.1.01

A Combined SAXS and NMR Analysis of the Partially Unfolded State of the Cataract-Causing V75D Mutant of Human  $\gamma$ D-Crystallin. Matthew Whitley, Angela Gronenborn, Jonathan Bartko, Zhaoyong Xi, Min G.

09:20-09:40AM 3.1.1.02

Powder Diffraction of Technetium at Non-Ambient Conditions. Daniel S. Mast, Eunja Kim, Emily Siska, Frederic Poineau, Kenneth R. Czerwinski, Barbara Lavina, Paul M. Forster.

09:40-10:00AM 3.1.1.03

High Pressure *in situ* Diffraction Study of  $A_2M_3O_{12}$  Compounds. Jennifer N. Gadiant, Cora Lind-Kovacs, Xiaodong Gao, Lindsay Young.

10:00-10:30AM Coffee Break

10:30-10:50AM 3.1.1.04

Snapshots of Ligand Entry, Malleable Binding, and Induced Helical Movement in P-glycoprotein. Aaron P. McGrath, Paul Szcwzyk, Houchao Tao, Mark Villaluz, Steven D. Rees, Sung Chang Lee, Rupak Doshi, Ina L. Urbatsch, Qinghai Zhang, Geoffrey Chang.

10:50-11:10AM 3.1.1.05

*Serum albumin* - the Metal Binding Hub. Katarzyna B. Handing, Wladek Minor,

Maksymilian Chruszcz, Ivan G. Shabalín.

11:10-11:30AM 3.1.1.06

Towards Improved Crystallography Through Molecular Dynamics. Pawel A. Janowski, David Case, Tom Terwilliger, Pavel Afonine, James Holton.

11:30-11:50AM 3.1.1.07

Structure and Function in the Acetoacetate Decarboxylase-Like Superfamily. Lisa Mueller, Nicholas Silvaggi.

11:50-12:00PM 3.1.1.08

Micro-Electron Diffraction (Micro-ED) Structure Determination of Type II Diabetes-Related Peptides. Pascal A. Krotee, Tamir Gonen, David S. Eisenberg, Lin Jiang, Brent Nannenga, Johan Hattne, Dan Shi, Francis Reyes, Duilio Cascio, Michael Sawaya, Jose A. Rodriguez.

### 3.1.2 Local Structure and Complex Materials

Graham King, James Neilson, Presiding Independence AB

09:00-09:20AM 3.1.2.01

Insights into Structural and Chemical Evolution in Novel Energy Storage Materials Using Hard X-Rays. Olaf J. Borkiewicz, Karena W. Chapman, Peter Chupas, Kamila M. Wiaderek.

09:20-09:40AM 3.1.2.02

Pair Distribution Function analysis for position resolved *in situ* studies of heterogeneous materials. Kirsten M. Jensen, Simon J. Billinge.

09:40-10:00AM 3.1.2.03

Local-Structure Refinements Using Multiple Measurement Techniques. Igor Levin.



Service & SmMolecules joint SIG Meeting .....	12:00pm.....	Independence CD
Small Angle Scattering SIG Meeting .....	12:00pm.....	Philadelphia North
Meet-the-Editor-in-Chief, International Tables.....	03:00pm.....	IUCr Booth 302
Business Meeting for ACA Members .....	05:00pm.....	Philadelphia North
Poster Session T .....	05:30pm.....	Liberty Ballroom

**10:00-10:50AM Coffee Break**

**10:50-11:10AM 3.1.2.05**

Multiply Twinned Nanoparticles and Interrelated Nanosheets: Nanostructure Studies Beyond the Unit Cell. Katharine Page, Edwin Fohtung, Heinz Nakotte, Corinne Silkwood, Daniel Olds, Hsiu-Wen Wang.

**11:10-11:30AM 3.1.2.06**

An Exotic Ruthenium Oxide Stabilized as a Nanocrystalline Glass. Martin D. Donakowski, Irina R. Pala, Paul A. DeSario, Christopher N. Chervin, Jeffrey W. Long, Debra R. Rolison.

**11:30-11:50AM 3.1.2.07**

Local and Average Structures of Complex Cation-Ordered Oxides,  $\text{LaBaMn}_2\text{O}_5$  and  $\text{Ba}_2\text{Y}_{0.5}\text{Fe}_{1.5}\text{O}_5$ . Corey Thompson.

**3.1.3 Hot Structures I  
Intracellular Protein Regulons**

Hyun-Joo Nam, Yi Tian Ting, Presiding

Freedom Ballroom

Funding for this session provided, in part, by TTP LabTech

**09:00-09:40AM 3.1.3.01**

Crystal Structure of the COP9 Signalosome - A Master Regulator of Intracellular Protein Degradation. Richard Bunker.

**09:40-10:00AM 3.1.3.02**

The 2.2 Å X-ray Crystal Structure of the Cytoplasmic Domain of the Inner Membrane Sigma Regulator, PupR, Reveals a Potential Helical Dimer. Christopher L. Colbert, Sangita Sinha, Srinivas Chakavarthy, Huaying Zhao, David B. Neau, Jaime Jensen.

**10:00-10:30am Coffee Break**

**10:30-11:00AM 3.1.3.03**

The Structure and Regulation of Human Muscle  $\alpha$ -actinin. Kristina Djinnovi-Carugo, Euripedes de Almeida Ribeiro, Nikos Pinot-

sis, Andrea Ghisleni, Anita Salmazo, Petr V. Konarev, Julius Kostan, Bjoern Sjoebloom, Claudia Schreiner, Anton A. Polyansky, Eirini A. Gkougkoulia, Mark R. Holt, Finn L. Aachmann, Bojan Zagrovc, Enrica Bordignon, Katharina F. Pirker, Dmitri I. Svergun, Mathias Gautel.

**11:00-11:20AM 3.1.3.04**

Structural and Functional Characterization of a Novel Complement Inhibitor from the *Leishmania* vector *Lutzomyia longipalpis*. Oluwatoyin Asojo, Bin Zhan, Jesus Valenzuela, Zhu Yun Liu, Alan Kelleher.

**11:20-11:40AM 3.1.3.05**

Structural Analysis of Inositol Pyrophosphate Kinases Uncovers Opportunities for Probe Development. Huanchen Wang.

**11:40-12:00PM 3.1.3.06**

An Unexpected Duo: Rubredoxin Binds Nine TPR Motifs to Form LapB, an Essential Regulator of Lipopolysaccharide Synthesis. Chelsy C. Prince, Zongchao Jia.

**3.1.4 Standard Practices in  
Crystallography I: Data Collection  
Strategies**

Peter Müller, Presiding

Independence CD

Funding for this session provided, in part, by Bruker, AXS

**09:00-09:30AM 3.1.4.01**

The Challenges of Soft X-rays: Data Collection Above 3 Å Wavelength. Dorothee C. Liebschner, Toshiya Senda, Yusuke Yamada, Miki Senda, Naohiro Matsugaki.

**09:30-10:00AM 3.1.4.02**

Fast Sative-SAD Phasing for Routine Macromolecular Structure Determination. Tobias Weinert, Vincent Olieric, Ezequiel Panepucci, Meitian Wa.

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### 10:00-10:30AM Coffee Break

#### 10:30-11:00AM 3.1.4.03

Tricks for Success using Zinc SAD Phasing. Chelsy C. Prince, Zongchao Jia.

#### 11:00-11:30AM 3.1.4.04

Theory and Practice in X-ray Diffraction Data Processing. Dominika Borek, Zbyszek Otwinowski, Wladek Minor, Marcin Cymborowski.

### 11:30-01:30pm Lunch Break

#### 01:30-02:00PM 3.1.4.05

Filling the Gaps: Data Collection Strategies for Collecting Diffuse Scatter and Bragg Data from Low Symmetry Space Groups. Mitchell D. Miller, George N. Phillips.

#### 02:00-02:30PM 3.1.4.06

Back to the Future: Revisiting and Improving Interleaved Protocols for Experimental Phasing, from Design to Processing. Gerard Bricogne, Clemens Vornrhein, Peter Keller, Wlodek Paciorek, Claus Flensburg.

#### 02:30-03:00PM 3.1.4.07

Data Collection Strategy for Macromolecules. Zbigniew Dauter.

### 03:00-03:30PM Coffee Break

#### 03:30-04:00PM 3.1.4.08

Fast Screening and Data Collection with the PHOTON 100 Detector. Bruce C. Noll.

#### 04:00-04:30PM 3.1.4.09

Case Specific Optimization of Data Collection Strategy. Leo H. Straver.

#### 04:30-05:00PM 3.1.4.10

Data Scaling with SADABS and TWINABS. George M. Sheldrick.

## 3.1.5 Structural Modeling for SAS

Tomas Weiss, Xiaolin Cheng, Presiding  
Philadelphia North

#### 09:00-09:30AM 3.1.5.01

Joining Neutron Scattering and Simulations for Complex Biomembranes. Xiaolin Cheng.

#### 09:30-10:00AM 3.1.5.02

Massively Parallel Computation for Small Angle Scattering. Hailiang Zhang, Joseph E. Curtis, Emre Brookes.

### 10:00-10:30AM Coffee Break

#### 10:30-11:20AM 3.1.5.03

Probing the Spatial Organization of Lipid Membranes with SANS. Frederick A. Heberle, John Katsaras, Georg Pabst, Drew Marquardt, Barbara Geier, Milka Doktorova, Viničius N. Anghel.

#### 11:20-11:40AM 3.1.5.04

Functional Cycle of a Eukaryotic Ribonuclease III: Solution Structures of *Saccharomyces cerevisiae* Rnt1p. He Song, Xinhua Ji, Yun-Xing Wang, Xianyang Fang.

#### 11:40-12:00PM 3.1.5.05

Structural Analysis of the *E. coli* Pol III Clamp Loader Sliding Clamp Complex. Farzaneh Tondnevis, Robert McKenna, Linda Bloom, Thomas Weiss, Tsutomu Matsui.

## 3.2.1 Important Science from Small Molecule Structures

Larry Falvello, Paulina Gonzalez, Presiding  
Philadelphia South

*Funding for this session provided, in part, by Crystallographic Resources*

#### 01:30-01:45PM 3.2.1.01

The Valence Multipole Model, Using Small Molecules to Create a New Bond Energy Expression for Molecular Mechanics. Matthew C. Wander, Charles Andros, Barry R. Bickmore.

#### 01:45-02:00PM 3.2.1.02

Molecular Magnets Combining Molecular, Nuclear and Magnetic Chirality. Javier Campo, Katsuya Inoue, Garry J. McIntyre, Cristina Saenz de Pipaon, Fernando Palacio.

**02:00-02:20PM** **3.2.1.03**  
Single Crystal to Single Crystal Transition of a Spin Crossover Material: Observation & Analysis. Christine M. Beavers, Jose Sanchez Costa, Guillem Aromi.

**02:20-02:40PM** **3.2.1.04**  
Single-crystal to Single-crystal Structural and Chemical Transformation of an Iron-based Molecular Electrocatalyst for Hydrogen Oxidation and Production. Xiaoping Wang, Tianbiao Liu, R. Morris Bullock.

**02:40-03:00PM** **3.2.1.05**  
Experimental Establishment of Mother-Daughter Orientation Relationships and Twinning Effects in Phase Transitions: A Great Legacy from Jack Gougoutas and Peggy Etter. Bruce M. Foxman, Aaron R. Gell, Onkei Tai, Shai R. Posner, Anthony H. Nguyen, Logan C. Lorson.

**3:00-3:30PM Coffee Break**

**03:30-03:50PM** **3.2.1.06**  
Surveying the Higher Dimensions of the Aperiodic Composite Nonadecane/urea. Garry J. McIntyre, Bertrand Toudic, Marie-Hélène Lemée-Cailleau.

**03:50-04:10PM** **3.2.1.07**  
A View on Electron Density Maps from Computational Homogeneous Catalysis. Felio Maseras.

**04:10-04:30PM** **3.2.1.08**  
Bromine - Bromine Bond Formation in the Cocrystallization of C70 with Bromobenzenes. Marilyn Olmstead, Joseph Wescott, Alan Balch, Susanne Chen, Kamran Ghiassi.

**04:30-05:00PM** **3.2.1.09**  
Important New Discoveries in Nanosized Homo-/Hetero-Palladium CO/PR<sub>3</sub> Clusters with Unexpected Implications. Lawrence F. Dahl, Sergei A. Ivanov, Evgueni G. Mednikov, Jeremiah D. Erickson.

## **3.2.2 Powder Pair Distribution Function and Pharmaceuticals**

**Simon Billinge, Peter Stephens, Presiding**  
**Independence AB**

**01:30-02:00PM** **3.2.2.01**  
Amorphous or Nanocrystalline? Advances in the Total Scattering Pair Distribution Function Methods for Characterizing Amorphous and Nanocrystalline Pharmaceuticals. Simon Billinge.

**02:00-02:30PM** **3.2.2.02**  
In House and Synchrotron Based Atomic PDF Studies on Non-crystalline Drugs: Is There Room for Both? Valeri Petkov.

**02:30-03:00PM** **3.2.2.03**  
Insights into the Recrystallization Behavior of Amorphous and Crystalline Lactose by Total Scattering Pair Distribution Function Analysis (TSPDF) and Solid State Nuclear Magnetic Resonance Spectroscopy (SSNMR). Eugene Cheung, Peter Quan, Simon Billinge, Maxwell W. Terban.

**3:00-3:30PM Coffee Break**

**03:30-04:00PM** **3.2.2.04**  
Structure Analysis of Molecular Systems using Atomic Pair Distribution Function. Pavol Juhas, Simon Billinge, Martin U. Schmidt, Dragica Prill.

**04:00-04:30PM** **3.2.2.05**  
Characterization and Structural Assessment of Pharmaceutical Solids by Total Scattering. Ahmad Y. Sheikh.

**04:30-05:00PM** **3.2.2.06**  
Crystal Structures of Large-Volume Commercial Pharmaceuticals with Z'<sup>></sup>1. James Kaduk, Thomas Blanton, Amy Gindhart, Kai Zhong, Robert Papoular, Joel Reid.

## **3.2.3 Hot Structures from Membrane Systems**

**David Lodowski, Presiding**  
**Freedom Ballroom**

**01:30-02:00PM** **3.2.3.01**

## TUESDAY, JULY 28

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A Scissor Blade-like Closing Mechanism Implicated in Transmembrane Signaling in a Bacteroides Hybrid Two-component System. Elisabeth C. Lowe, Arnaud Baslé, Mirjam Czjzek, Susan Firbank, David Bol.

**02:00-02:30PM** **3.2.3.02**  
The Glove-like Structure of the Integral Membrane Protein TatC. William Clemons Jr.

**02:30-03:00PM** **3.2.3.03**  
A Hot Structure With a Cold Start. AlgE v.2. Martin Caffrey.

### **3:00-3:30PM Coffee Break**

**03:30-04:00PM** **3.2.3.04**  
High-resolution Crystal Structures of the Influenza AM2 Proton Channel: Insights Into Water Networks. Jessica Thomaston, Rachel Woldeyes, Ayumi Yamashita, Eriko Nango, Rie Tanaka, James Fraser, William DeGrado.

**04:00-04:20PM** **3.2.3.05**  
A Conserved Solvent Network in the Transmembrane Region of Activated Osin is Essential for Receptor Activation. Elise Blankenship, David T. Lodowski.

**04:20-04:40PM** **3.2.3.06**  
Structural and Mechanistic Insights into the Recruitment of Talin by RIAM in Integrin Signaling. Yu-Chung Chang, Jinhua Wu, Edna Cukierman, Tejash Patel, Mark Brennan, Janusz Franco-Barraza, Hao Zhang.

**04:40-05:00PM** **3.2.3.07**  
Tie2 Receptor Dimerization is Mediated by its Extracellular FNIII Domains. Jason O. Moore, Mark A. Lemmon, Kathryn M. Ferguson.

### **3.2.4 Standard Practices in Crystallography II: Data Collection Strategies**

Peter Müller, Presiding  
Independence CD

**01:30-02:00PM** **3.1.4.05**  
Filling the Gaps: Data Collection Strategies for Collecting Diffuse Scatter and Bragg Data from Low Symmetry Space Groups. Mitchell D. Miller, George N. Phillips.

**02:00-02:30PM** **3.1.4.06**  
Back to the Future: Revisiting and Improving Interleaved Protocols for Experimental Phasing, from Design to Processing. Gerard Bricogne, Clemens Vonrhein, Peter Keller, Wlodek Paciorek, Claus Flensburg.

**02:30-03:00PM** **3.1.4.07**  
Data Collection Strategy for Macromolecules. Zbigniew Dauter.

### **3:00-3:30PM Coffee Break**

**03:30-04:00PM** **3.1.4.08**  
Fast Screening and Data Collection with the PHOTON 100 Detector. Bruce C. Noll.

**04:00-04:30PM** **3.1.4.09**  
Case Specific Optimization of Data Collection Strategy. Leo H. Straver.

**04:30-05:00PM** **3.1.4.10**  
Data Scaling with SADABS and TWINABS. George M. Sheldrick.

### **3.2.5 Evolving Techniques for SAS**

Cheng Wang, Michal Sabat, Presiding  
Philadelphia North

*Funding for this session provided, in part, by Anton Paar*

**01:30-01:55PM** **3.2.5.01**  
SAXS/WAXS, Crystallisation and Sample Robustness for Time Resolved Experiments. Wim Bras.

**01:55-02:20PM** **3.2.5.02**  
Recent Developments in Laboratory SAXS Instrumentation - What Is Possible Today? Peter Mario Worsch, Andreas Keilbach, Gerd Langenbacher.

**02:20-02:40PM** **3.2.5.03**  
SAXS Insights into Meso- and Nano-Structure Dynamics in Iron-Based Electrochemical

Conversion Reactions. Kamila M. Wiaderek, Karena W. Chapman, Peter Chupas.

**02:40-03:00PM** **3.2.5.04**  
SAXS, Polymer Nanocomposites, Wetting Phase Transitions, and Nanoparticle Dispersion, What have we Learned so Far? David Green.

**3:00-3:30PM Coffee Break**

**03:30-03:55PM** **3.2.5.05**  
Integration of SAXS with Complementary Techniques for Structural Characterization of Large Biomolecular Complexes. Tobias Madl.

**03:55-04:20PM** **3.2.5.06**  
Microstructure Evolution of Thin Films Examined by GISAXS with Tender X-rays. Hiroshi Okuda, Noriyuki Igarashi, Nobutaka Shimizu, Hiroki Ogawa, Shin-ichi Sakurai, Yoshinori Kitajima, Takayoshi Yamamoto.

**04:20-04:40PM** **3.2.5.07**  
Characterizing Directed Self Assembly Block Copolymers with Soft X-rays. Daniel F. Sunday, R. Joseph Kline.

**04:40-05:00PM** **3.2.5.08**  
Polarized Resonant X-ray Scattering to Probe Orientation and Alignment of Organic Molecules. Brian A. Collins.

**3.3.1 Evening Session on Diversity**  
Krystle McLaughlin, Presiding  
Freedom Ballroom

**05:00-06:00PM** **3.3.1.01**  
Does Diversity Training Work? Catherine L.

Drennan, MIT/HHMI.

**06:00-06:20PM** **3.3.1.02**  
Stephanie B. Wort, New York Academy of Sciences.

**06:20-06:40PM** **3.3.1.03**  
Diversity in STEM: Tips, Resources, and Opportunities from AAAS. Dione L. Rossit, American Association for the Advancement of Science.

**Business Meeting  
for all ACA Members**

**5:00pm Freedom Ballroom**

**All are welcome and strongly  
encouraged to attend**

# WEDNESDAY, JULY 29

Registration Desk .....	7:30am .....	Liberty Ballroom Foyer
Speaker Ready Room .....	7:30am .....	Salon 8
Council Meeting Room .....	7:30am .....	Salon 5/6
MOVIE: "The Mystery of the Giant Crystals" .....	12:00pm .....	Independence AB
Awards Banquet (ticket required) .....	6:30pm .....	Liberty Ballroom

## P4 Plenary Lecture:

Chris Cahill, presiding

Freedom Ballroom

08:00-08:45am

P4.01

The Impact of Crystals and Crystallography in Art and Culture. Juan M. Garcia-Ruiz.

Join Dr. Garcia-Ruiz at 12:00PM for a free viewing of the documentary "The Mystery of the Giant Crystals" in Independence AB

## 4.1.1 Structural Glycobiology

David Rose, Michael James, Presiding

Freedom Ballroom

09:00-09:25AM

4.1.1.01

$\beta$ -lactam Antibiotic Resistance and the Bacterial Peptidoglycan Recycling Pathway. Brian L. Mark.

09:25-09:45AM

4.1.1.02

Guided Model-Building of N-linked Carbohydrates. Paul Emsley.

09:45-10:00AM

4.1.1.03

Engineering FlgJ to Study the Catalytic Mechanism of Family 73 Glycoside Hydrolases. Patryk Zaloba, Ben A. Bailey-Elkin, Brian L. Mark.

10:00-10:30AM Coffee Break

10:30-11:00AM

4.1.1.04

Carbohydrate-recognising Proteins: Structural Features and Challenges in Inhibitor Design. Helen Blanchard.

11:00-11:20AM

4.1.1.05

Crystal Structures of LpoA, a Peptidoglycan Synthase Activator from *Haemophilus influenzae*. Mark A. Saper, Kathleen C. Wissner, J Vijayalakshmi, Karthik Sathiyamoorthy.

11:20-11:40AM

4.1.1.06

Feeding our Gut Microbes: Structural Insights into Sugar Digestion in the Human Colon. Marcia Chaudet, David Rose.

11:40-12:00PM

4.1.1.07

Novel Structures of *Xenopus laevis* and Human X-type Lectins Reveal Mechanism of Carbohydrate Recognition. Kittikhun Wangkanont, Darryl A. Wesener, Katrina T. Forest, Laura L. Kiessli.

## 4.1.2 General Interest II

Peter Müller, Presiding

Independence CD

09:00-09:20AM

4.1.2.01

Structural Chemistry and Drug Discovery at Merck. Giovanna Scapin.

09:20-09:40AM

4.1.2.02

Development of the CheckMyMetal Server. Heping Zheng, Wladek Minor, Ivan G. Shabalina, David Cooper, Mahendra Chordia.

09:40-10:00AM

4.1.2.03

MolProbit's Ultimate Rotamer Library for Model Validation. Bradley J. Hintze, Jane S. Richardson, David C. Richardson.

10:00-10:30AM Coffee Break

10:30-10:55AM

4.1.2.04

Innovative Protein Crystallization Screens. Fabrice Gorrec.

10:55-11:20PM

4.1.2.05

A Comprehensive Strategy to Obtain High Quality Crystals. Miki Senda, Toshiya Senda.

11:20-11:40AM

4.1.2.06

The Structural Biology of the Origin of Life. Charles W. Carter.

**11:40-12:00AM** **4.1.2.07**  
Rfree: A Dinosaur Marked for Extinction? Du-  
san Turk, Jure Praznikar.

### **4.1.3 In the Service of Science: Experiences and Opportunities with Central Facility Services**

**Christine Beavers, Banumathi Sankaran, Presiding  
Philadelphia North**

**09:00-09:05AM Opening Remarks**

**09:05-09:40AM** **4.1.3.01**  
Structural Biology of Viral Proteins Critical  
for Glycan Recognition and Immune Evasion.  
Bidadi V. Prasad, Sreejesh Shanker, Banu-  
mathi Sankaran, Zana Muhaxhiri, Berenice  
Carrillo, Liya Hu.

**09:40-10:00AM** **4.1.3.02**  
BioMEX Solutions: An Expert Facility for  
Structure Solution in Macromolecular X-ray  
Crystallography. Ronan Keegan, Sapan Gan-  
dhi, Eugene Krissinel.

**10:00-10:30AM Coffee Break**

**10:30-11:05AM** **4.1.3.03**  
The Acetylcholine Binding Protein as a Tool  
for Drug Discovery: A Quest for Specificity.  
Todd T. Talley, Janet Bobango.

**11:05-11:30AM** **4.1.3.04**  
Beyond the Bottleneck: the User Programs  
and Avenues of Access to the MBC Beamline  
ALS4.2.2. Jay C. Nix.

**11:30-11:55AM** **4.1.3.05**  
Service Crystallography Modes on Beamline  
11.3.1 at the Advanced Light Source. Simon J.  
Teat, Christine M. Beavers, Kevin J. Gagnon.

### **4.1.4 Important Science from Small Molecular Structures Part II**

**Paulina Gonzalez, Alberto Albinati, Presiding  
Philadelphia South**

**09:00-09:20AM** **4.1.4.01**  
Structural Chemistry of Tetravalent Actinide-  
organic Based Compounds. Karah E. Knope.

**09:20-09:40AM** **4.1.4.02**  
Using X-ray Crystallography to Elucidate  
Ligand and Metal Oxidation States in Low-  
valent Uranium Complexes Bearing Redox-  
active Ligands. Suzanne C. Bart.

**09:40-10:00AM** **4.1.4.03**  
Structures and Properties of Metastable  
 $A_2BB'O_6$  Corundum Derivatives. Peter Ste-  
phens, Martha Greenblatt, David Walker, Ma-  
ria Retuerto, Man-Rong.

**10:00-10:30AM Coffee Break**

**10:30-10:45AM** **4.1.4.04**  
The Story of a Flexible Receptor: from Self-  
assembly Strategies to Successful Separation of  
Isomeric Dicarboxylic Acids. Ivica Djilovic.

**10:45-11:00AM** **4.1.4.05**  
A Reinvestigation of Ruthenium Chemistry:  
the Importance of X-ray Crystallography for  
Definitive Structural Characterization. Ka-  
mran Ghiassi, Michael Aristov, Alan Balch,  
Marilyn Olmstead.

**11:00-11:20AM** **4.1.4.06**  
Structural and Electronic Characterization  
of  $M^{n+}[Mo_2]^{4+}$  Complexes. Brian S. Dolinar,  
John F. Berry.

**11:20-11:40AM** **4.1.4.07**  
Crystal Packing in High-Z' Structures of Or-  
ganic Molecules. Carolyn P. Brock.

**11:40-12:00PM** **4.1.4.08**  
Important Science from 764,371 Small Mol-  
ecule Structures. Colin R. Groom, Peter A.  
Wood.

### **4.1.5 (Bio)Chemistry in the X-ray Beam**

**Sean McSweeney, Elspeth Garman, Presiding  
Independence AB**

**09:00-09:40AM** **4.1.5.01**  
Using Single Crystal Spectroscopy to your  
Advantage: the Case of the Missing Ferryl  
iron. Carrie M. Wilmot, Victor L. Davidson,  
Britt Hedman, Allen M. Orville, Riti Sarangi,

Babak Andi, Chao Li, Erik T. Yukl.

**09:40-10:00AM** **4.1.5.02**

Crystallographic Study for Estimation of the Valence of Four Mn Atoms in Oxygen-evolving Photosystem II using Anomalous Absorption Techniques. Yasufumi Umena, Nobuo Kamiya, Jian-Ren Shen, Keisuke Kawakami.

**10:00-10:30AM Coffee Break**

**10:30-11:10AM** **4.1.5.03**

Radiation Damage to Protein Crystals: Phenomenology, Mechanisms, and How to Reduce It at Next Generation Synchrotron Beamlines. Robert E. Thorne.

**11:10-11:30AM** **4.1.5.04**

Imaging Local Electric Fields Produced upon Synchrotron X-ray Exposure. Garth Simpson, Robert F. Fischetti, Michael Becker, Scott Toth, Justin Newman, Christopher Dettmar.

**11:30-11:50AM** **4.1.5.05**

Use of Chemical Restraints in Phenix. Nigel Moriarty.

## 4.2.1 General Interest III

Peter Mueller, Stacey Smith, Presiding  
Independence CD

**01:30-02:00PM** **4.2.1.01**

Celebrating the International Year of Crystallography with Crystal Growing Competitions. Ilia Guzei.

**02:00-02:20PM** **4.2.1.02**

Finding Your Place in the World - Using the CSD to Benchmark Your Research. Amy A. Sarjeant, Colin R. Groom, Peter A. Wood, Suzanna C. Ward, Seth Wiggin.

**02:20-02:40PM** **4.2.1.03**

Crystallographic Point Groups and Abstract Groups; Mathematical Crystallography. Maureen M. Julian.

**02:40-03:00PM** **4.2.1.04**

Expanding the Low-valent Chemistry of

Technetium Through Hydrothermal Synthesis. Paul M. Forster, Kenneth R. Czerwinski, Alfered P. Sattelberger, Frederic Poineau, William M. Kerlin.

**03:00-03:30PM Coffee Break**

**03:30-03:50PM** **4.2.1.05**

Molecular Crystals That Cannot Be Prepared in a Test Tube. Larry R. Falvello, Milagros Tomas, Isabel Mayoral, Elena Forcén-Véquez, Isabel T. Dobrinovitch.

**03:50-04:10PM** **4.2.1.06**

Practical Guidelines and Insights for the Crystalline Sponge Method. Timothy R. Ramadhar, Shao-Liang Zheng, Yu-Sheng Chen, Jon Clard.

**04:10-04:30PM** **4.2.1.07**

Native-SAD is Maturing. John P. Rose, Manfred Weiss, B.C. Wang.

**04:30-04:45PM** **4.2.1.08**

Vaterite Structure and Microstructure of Sturgeon Otoliths. Bryan C. Chakoumakos, Mikhail Feygenson, Ronald M. Bruch, Ryan Koenigs, Brenda M. Pracheil.

**04:45-05:00PM** **4.2.1.09**

The Monoclinic Form of the Rhabdophane Compounds: REEPO<sub>4</sub>·0.667 H<sub>2</sub>O. Adel Mesbah, Nicolas Dacheux, Stephanie Szenknect, Ilyes ben Kacem, Clemence Gausse, Erik Elkaim, Nicolas Clavier.

## 4.2.2 Cool Structures

Allen Oliver, Chris Durr, Presiding  
Philadelphia South

**01:30-02:00PM** **4.2.2.01**

The Influence of Chemistry and Topology on the High Pressure Behaviour of Hybrid Materials. The Influence of Chemistry and Topology on the High Pressure Behaviour of Hybrid Materials. Elinor Spencer, Christopher Cahill, Kory Carter, Nancy Ross.



**02:00-02:30PM** **4.2.2.02**  
Effect of Chemistry on the High-Pressure Behavior of Monazite, a Rare-Earth Phosphate. Karina M. Heffernan, Lynn Boatner, Elinor Spencer, Nancy Ross.

**02:30-03:00PM** **4.2.2.03**  
Borates: New Structural Types, Pseudo-Merohedral Twinning, and Disorder. Yulia Sevryugina, David M. Schubert, Doinita Neiner.

**03:00-03:30PM Coffee Break**

**03:30-04:00PM** **4.2.2.04**  
Structural Classifications in Inorganic Materials. Soorya N. Kabekkodu.

**04:00-04:30PM** **4.2.2.05**  
Metal Halides in Li-ion Batteries. Craig Bridges, Sheng Dai, Stephen Nagler, Arnab Banerjee, Gabriel M. Veith, Jonathan M. Powell.

**04:30-05:00PM** **4.2.2.06**  
Another year.... Patrick J. Carroll.

### **4.2.3 Structured Nucleic Acids**

**Eric Montemayor, Manal Swairjo, Presiding Independence AB**

*Funding for this session provided, in part, by Chemgenes, Hampton Research, Integrated DNA Technologies and MiTiGen*

**01:30-01:50PM** **4.2.3.01**  
Structural Comparison of HIV-1 Reverse Transcriptase Cross-Linked to a DNA Template-Primer at Two Different Sites. Sergio E. Martinez, Eddy Arnold, Kalyan Das.

**01:50-02:10PM** **4.2.3.02**  
Reading DNA Sequence by the Transcription Regulator PhoP. Shuishu Wang, Xiaoyuan He.

**02:10-02:30PM** **4.2.3.03**  
Mg-RNA Server: Automated Classification of Magnesium Binding Sites in RNA Crystal Structures. Ivan G. Shabalin, Wladek Minor, Katarzyna B. Handing, Heping Zheng.

**02:30-03:00PM** **4.2.3.04**  
Structural Metamorphosis of Human Amino-

acyl-tRNA Synthetases for Novel Functions. Min Guo.

**03:00-03:30PM Coffee Break**

**03:30-04:00PM** **4.2.3.05**  
Helical Repeats Hinder Direct Methods Structure Determination of Double-stranded RNA from Trypanosome RNA Editing. Blaine Mooers.

**04:00-04:30PM** **4.2.3.06**  
Crystal Structure of a Group II Intron Lariat. Navtej Toor.

**04:30-05:00PM** **4.2.3.07**  
Regulated Disruption and Re-assembly of U4/U6 di-snRNP During Splicing. Markus C. Wahl.

### **4.2.4 Imaging with X-rays and Electrons**

**Vivian Stojanoff, Dean Chapman, Presiding Independence AB**

**01:30-02:00PM** **4.2.4.01**  
A Comparison of Cryo Microscopy with X-rays and Electrons. Chris Jacobsen.

**02:00-02:20PM** **4.2.4.02**  
Sub-micron X-ray Beam Study of Human Hair. Vesna Stanic, Kenneth Evans-Lutterodt, Fabiano Emmanuel Montoro, Jefferson Bettini.

**02:20-02:40PM** **4.2.4.03**  
X-ray Topography Techniques for Imaging Defects and Strain in Crystalline Materials: Current Status and Future Prospects. Balaji Raghathamachar, Michael Dudley.

**02:40-03:00PM** **4.2.4.04**  
Applications of TEM for Evaluation and Optimization of Crystal and Nano Crystal Growth. Guillermo A. Calero, Aina Cohen, James F. Conway, Christopher O. Barnes, Guowu Lin, Hilary Stevenson.

**03:00-03:30PM Coffee Break**

## WEDNESDAY, JULY 29

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**03:30-04:00PM** **4.2.4.05**  
Coherent X-ray Scattering: Dynamics of Crowded Colloids and Other Stories. Andrei Fluerașu.

**04:00-04:20PM** **4.2.4.06**  
Tomographic Coherent X-ray Diffraction Imaging of Dentin Tissue Ultrastructure. Mariana Verezhak, Aurlien Gourrier, Marie Plazanet, Elsa Vennat, Manfred Burghammer, Britta Weinhausen, Federico Zontone, Yuriy Chushkin.

**04:20-04:50PM** **4.2.4.07**  
Diffraction Enhanced Imaging at the Biomedical Beamline at the Canadian Light Source. Dean Chapman.

### 4.2.5 Play it Cool? Ambient and Cryogenic Approaches

Doug Juers, James Fraser, Presiding  
Philadelphia North

*Funding for this session provided, in part, by MiTiGen*

**01:30-02:00PM** **4.2.5.01**  
Physics of Cryo- and Variable-Temperature Crystallography. Robert E. Thorne.

**02:00-02:20PM** **4.2.5.02**  
Crystal Mounting Method using Humid Air and Hydrophilic Glue Coating For Ambient and Cryogenic Experiments. Takashi Kumasaka, Masaki Yamamoto, Tohru Kataoka, Fumi Shima, Shigeyuki Matsumoto, Takashi Kawamura, Nobuo Kamiya, Yasufumi Umena, Naoto Yagi, Seiki Baba.

**02:20-02:40PM** **4.2.5.03**  
Morphological Characterization of Detergent-mediated Photosystem I (PS I)- Proteoliposome Formation. Hanieh Niroomand.

**02:40-03:00PM** **4.2.5.04**  
Vapor Diffusion Based Cryoprotection of Macromolecular Crystals. Douglas H. Juers, Christopher Farley.

**03:00-03:30PM Coffee Break**

**03:30-04:00PM** **4.2.5.05**  
Radiation Damage Effects on Protein Conformation at Room Temperature and 100K. Ana Gonzalez.

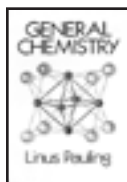
**04:00-04:30PM** **4.2.5.06**  
Exploiting the Virtues of Cryo-crystallography and *in situ* Data Collection at Beamline I24. Danny Axford.

**04:30-05:00PM** **4.2.5.07**  
Discovering Coupled Conformational Heterogeneity in Proteins by Multitemperature Crystallography and Multiscale Modeling. Daniel Keedy, James S. Fraser, Jim Wells, Justin Rettenmaier.

## THURSDAY, JULY 30

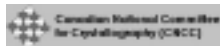
Planning Session for  
2016 Denver Meeting

8:30AM Horizons Ballroom (on the rooftop)



## Pauling Poster Prize, Canadian and IUCr Poster Prize

The Pauling Poster Prize established by the ACA and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of \$250, a complimentary banquet ticket, and a copy of a Linus Pauling book. An additional Pauling Prize sponsored by the Canadian Div. of the ACA and the Canadian National Committee, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory.



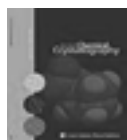
## IUCr Poster Prize

The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.



## Journal of Chemical Crystallography Poster Prize

The best graduate or undergraduate poster presentation in the area of chemical crystallography or small molecule structure determination and analysis is sponsored by Springer's Journal of Chemical Crystallography [www.springer.com](http://www.springer.com). The winner will receive their personal choice of books from Springer's extensive portfolio of titles.



## Journal on Structural Dynamics Poster Prize

The prize of \$250 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.

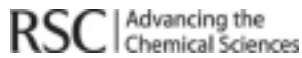
## RCSB Protein Data Bank Poster Prize

This prize recognizes a student poster presentation involving macromolecular crystallography. The award will be 2 educational books that will be mailed to the winner after the meeting. An announcement will appear on the RCSB PDB website and newsletter.



## CrystEngComm Poster Prize

CrystEngComm (published by the Royal Society of Chemistry) is very pleased to sponsor a prize to be awarded to the best graduate or undergraduate poster presentation in the area of crystal engineering/supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted on the CrystEngComm website ([www.rsc.org/Publishing/Journals/CE/about.asp](http://www.rsc.org/Publishing/Journals/CE/about.asp)) shortly after the conclusion of the meeting.



## Oxford Cryosystems Low Temperature Poster Prize

This prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.



## Taylor & Francis Biomolecular Crystallography Poster Prize

This prize is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The winner will receive



Bernhard Rupp's book Biomolecular Crystallography donated by the Taylor

& Francis Group and will be announced at the banquet on Wednesday.

### POSTER HANGING INSTRUCTIONS

Posters beginning with S should be assembled before 11:00am on Sunday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with M should be assembled before 11:00am on Monday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with T should be assembled before 11:00am on Tuesday and be removed at the conclusion of the poster session at 7:30pm.

**Please be present at your poster from 5:30 - 7:30pm on the day to which you are assigned and remove your poster at the end of the session.**

### Sunday Posters

Poster session sponsored by



#### S01

A Novel Approach to Overcome Antibiotic Resistance by Targeting ERA, an Essential GTPase That Couples Cell Growth with Cell Division. Vandana Kumari, Xinhua Ji, Donald Court, David S. Waugh, Genbin Shi, Joseph Tropea.

#### S02

A Unique Human Mycoplasma Protein that Generically Blocks Antigen-Antibody Union. Xueyong Zhu, Ian A. Wilson, Richard A. Lerner, Andrew B. Ward, Helen J. Kim, Travis Nieuwsma, Rajesh K. Grover.

#### S03

Bacterial Hydrocarbon Biosynthesis: Elucidating the Role of Glu117 $\beta$  in the Mechanism of OleA. Matthew R. Jensen.

#### S04

Beclin 2 Interacts with Atg14 Through a Metastable Coiled-coil to Regulate Autophagy. Minfei Su, Sangita Sinha, Christopher L. Colbert, David Neau, Yue Li.

#### S05

Biophysical Analysis of a Natively Folded

VDAC. Fraser G. Ferens, Deborah A. Court, Joerg Stetefeld, George Orriss.

#### S06

Charge-transfer Complexes Between Bis(arene)iron(II) Salts and Aromatic Compounds: Removing the Cobwebs from an Old Story. Mark W. Bezpalko, Bruce M. Foxman.

#### S07

Chiral Channels in Molecular Co-Crystals: Unexpected Structures that Arise from the Co-crystallization of 2,4,6-tris(4-X-phenyl)arenes. Ren Wiscons, Jesse Rowsell, Matthias Zeller, Holden Lai.

#### S08

CIPC Interacts with Exon19 of CLOCK Protein to Function as an Additional Negative-Feedback Regulator in Circadian Rhythm. Zhiqiang Hou, Hong Zhang, Lijing Su.

#### S09

Conformational Flexibility in a Conserved Beclin 1 Region Essential for Starvation-mediated Autophagy. Yang Mei, Sangita Sinha, Christopher L. Colbert, Srinivas Chakravarthy, Ruslan Sanishvili, Minfei Su, Karen Glover.

#### S10

Crystal Structure and Receptor Binding of the Haemagglutinin from Human-infecting H10N8 Influenza Virus. Heng Zhang, Ian A. Wilson, James Paulson, Ryan McBride, Wenli Yu, Xueyong Zhu, Netanel Tzarum, Robert de Vries.

**S11**

Crystal Structure of a Drug Target Midazole-glycerol-phosphate Dehydratase (IGPD) from *Mycobacterium tuberculosis*. Mohd S. Ahang.

**S13**

Crystal Structures of Native and Mutant HIV-1 Capsid Proteins Reveal Molecular Details of Interactions with Ligands and Structural Basis of Capsid Stability. Anna T. Gres.

**S14**

Education of the Active Site of Bovine Liver Catalase with X-Rays. Osvaldo Gomez.

**S15**

Effect of Cations and pH on Neurospora crassa CDHIIA Dimensions Investigated by Small Angle X-ray Scattering. Annette M. Bodenheimer, Flora Meilleur.

**S16**

Effect of Environmental Pollutants on Xenobiotic Regulation via P-glycoprotein (P-gp). Steven Rees, Geoffrey Chang, Aaron P. McGrath.

**S17**

Effect of Protein Crystal Hydration on Side Chain Conformation and Heterogeneity. Hakan Atakisi, Robert E. Thorne, Jesse Hopkins, David Moreau.

**S18**

Entropy or Enthalpy or Both, that is the Question: A Fresh Look Beyond the Asymmetric unit of Protein Crystals. Yancho Dewedjiev, Dusan Turk, Jure Praznikar.

**S19**

Enzyme Discovery for Natural Product Biosynthesis. Hongnan Cao, George N. Phillips Jr., The 3 Northeast Center for Structural Genomics, The Midwest Center for Structural Genomics, The Center for Natural Product Biosynthesis.

**S20**

H...H Clashes in Published Carboxylic Acid Structures. Carl H. Schwalbe.

**S21**

High Resolution Crystal Structures of Antiviral, Glycosylated Y3 Protein from the Fungus *Coprinus comatus*. Kunhua Li, Steven D. Bruner, Yousong Ding, Peilan Zhang, Guang Yang.

**S22**

*In silico* Characterization and Visualization of a Protein of Unknown Function (4GHB) that May Have Enzymatic Activity. Paul A. Craig, Herbert J. Bernstein, Kaneisha Cherry-Irby.

**S23**

*In silico* Studies of the Function of Crystal Structure of a Porin-like Protein (BACU-NL\_01323) from *Bacteroides uniformis* ATCC 8492 at 2.32 Å Resolution. Limone Rosa, Paul A. Craig, Herbert J. Bernstein.

**S24**

Intercalating Dyes for Enhanced Contrast in Second Harmonic Generation Imaging of Protein Crystals. Nicole Scarborough, Garth Simpson, Nicholas Pogradichniy, Justin Newman.

**S25**

Modeling the Crystal Structure and Ion Exchange Mechanisms of Rare Earth Elements into zorite. Joseph Chappell, Aaron Celestian.

**S26**

Molecular Interactions Within the Crumbs Cell Polarity Complex. Marina E. Ivanova, Neil Q. McDonald, Barry J. Thompson, Svend Kjaer, Andrew G. Purkiss, Nicola O'Reilly, Georgina C. Fletcher, Peter Saiu.

**S27**

Nicotinamide Adenine Dinucleotide Biosynthesis in *Streptococcus pyogenes*. William T. Booth, Trevor L. Morris, Lesa R. Offermann, Maksymilian Chrusz.

**S28**

Non-canonical Hydrogen Bonding to AdoMet is a Common Feature of AdoMet-dependent Methyltransferases. Robert Fick, Steve

## Posters-S

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Scheiner, Dean A. Myles, Flora Meilleur, Ryan A. Mehl, Hazel M. Holden, Raymond Triebel.

### S29

Novel Comprehensive Approaches to Optimize Crystal Growth and Nanocrystal Sample Preparation using Transmission Electron Microscopy. Christopher O. Barnes, Guillermo A. Calero, Aina Cohen, Guowu Lin, Elena Kovaleva, Hilary Stevenson.

### S31

Pressure Induced Structural Transition in  $\text{Ho}_{0.5}\text{Y}_{1.5}\text{Ti}_2\text{O}_7$  by Synchrotron XRD and Raman Experiments. Melanie A. White, Jesse S. Smith, Andrew Cornelius, Michael Pravica, Brian Light, Jason Baker, Ravhi S. Kumar.

### S32

Protein Electron Transfer Complexes During the Initiation of Polychlorinated Biphenyl Degradation Investigated by Small-Angle X-ray Scattering. Jaime Jensen, Christopher L. Colbert, Sangita Sinha, Srinivas Chakravarthy, David B. Neau, Karen Glover, Zachery Staskywicz, Benjamin LeVahn.

### S33

REST APIs for Searching and Accessing PDB and EMDB. Sameer Velankar, Gerard Kleywegt, Ardan Patwardhan, Aleksandras Gutmanas, John Berrisford, Michael Wainwright, Glen van Ginkel, Saqib Mir, Ingvar Langerstedt, Younes Alhroub, Manuel Fernandez Montecelo, Eduardo Sanz-Garcia, Swanand Gore, Jose Dana.

### S34

Self-Healing Dynamics in Ultra-High Temperature Carbide-Diamondoid Nuclear Fuels. Boris Udovic.

### S35

Preparation And Properties of New Group-13 Based Metal-organic Frameworks. Daniel Reinares-Fisac, L.M. Aguirre, N. Snejko, M. Iglesias, E. Gutierrez-Puebla, F. Gandara, M. Monge.

### S36

Structural and Functional Characterizations of Solute Binding Proteins by Differential Scanning Fluorimetry and Crystallography. Umesh Yadava, Steven C. Almo, J. A. Gerlt, K. L. Whalen, R. D. Siedel, J. Love, Rafael Toro, N.F. Al-Obaidi, Matthew W. Vetting.

### S37

Structural and Optical Properties Study of Nanocrystalline Si (nc-Si) Thin Films Deposited on Porous Aluminum by PECVD. Skander Ktifa.

### S38

Structural Basis for Sequestration of Anti- $\sigma 70$  Factor Rsd from  $\sigma 70$  by Dephosphorylated HPr. Si-Hyeon Um.

### S39

Structural Basis for the Substrate Specificity of Periplasmic Glucose Binding Protein ppGBP from *Pseudomonas putida* CSV86. Suman Pandey, Prasejnit Bhaumik, Arnab Modak, Huanchen Wang.

### S40

Structural Development of Enzyme Toolbox for Natural Product Biosynthesis. Fengbin Wang, George N. Phillips Jr., Jon Thorson, Craig Bingman, Kate Helmich, Mitchel Miller, Eileen Brady, Weijun Xu, Shanteri Singh.

### S41

Structural Investigation of Polyketide Synthase Architecture. Meredith Skiba, Janet L. Smith, David H. Sherman, William H. Gerwick, Jonathan R. Whicher.

### S42

Structural Studies of FoxC2 DNA Binding Domain. Shichang Li, Hyun-Joo Nam, Shruti, Lagnajeet Pradhan.

### S43

Structural Studies of the Fused PqqCD Enzymes in *Methylobacterium extorquens* offer Insights into PqqD Function. Robert L. Evans.

**S44**

Structure of GrIR and GrIR-GrIA Complex that Provide Mechanistic Insight into a Regulatory Module for the Virulence of Enteropathogenic and Enterohemorrhagic *Escherichia coli*. Jobichen Chacko, J Sivaraman, Abhilash Padavannil.

**S45**

Structure-Based Discovery of Allosteric HIV Integrase Inhibitors. Daniel Klein, Jay Grobler, Tracy Diamond, Daniel Krosky, Doug Beshore, Antonella Converso, Kartik Narayan, Sujata Sharma, John Reid, Sangita Patel, John Sande.

**S46**

Structure-Based Drug Design of Isoform Specific Carbonic Anhydrase Inhibitors. Avni Bhatt, Robert McKenna, Claudiu Supuran, Mariangela Ceruso, Benedetta Cornelio, Carrie L. Lomelino, Brian P. Mahon.

**S47**

Synthesis and X-ray Characterization of Cobalt Phosphide Nanorods for Oxygen Reduction Reaction. Vicky Doan-Nguyen, Christopher B. Murray, Karen Winey, Jing Li, Dong Su, Rahul Agarwal, Edward B. Trigg, Sen Zhang.

**S48**

Template-Directed Nucleation of Diarylurea Polymorphs. Marina A. Solomos, Jennifer A. Swift, Christina Capacci-Daniel, Serena Seshadri.

**S49**

Templation Effects and Novel ZIF Structures by Solid State SSynthesis. Ivana Brekalo.

**S51**

The First X-ray Crystal Structure of Full-length Mammalian Phenylalanine Hydroxylase. Emilia C. Arturo, Patrick J. Loll, Eileen K. Jaffe, Annie Heroux, Thomas Scary, Ursula Ramirez.

**S52**

The Incorporation of Polyaromatic Hydrocarbons into an S-layer protein of the Hyperthermophilic Archaeon *Staphylothermus marinus*. Matthew D. McDougall, Jorg Stetefeld, Gregg Tomy, Thor Halldorson, Fraser Ferens, Markus Meier.

**S53**

The Role of Avidity in Tankyrase-1 Substrate Selection. Travis J. Eisemann, John M. Pascal, Swati Roy, Marie-France Langelier, Marie-France Langelier.

**S54**

The Roles of Active Site Residues and Water Molecules for Ligand Orientation in Arabidopsis dUTPase. Noriko Inoguchi, Hideaki Moriyama.

**S55**

The Supramolecular Self Assembly of the Uranyl Tetrahalide and Isothiocyanate Tectons: A Step toward Understanding the Underlying Factors that Govern Assembly, Speciation and Properties. Robert G. Surbella.

**S56**

The wwPDB Deposition and Annotation System. Brian P. Hudson, the wwPDB team, Stephen K. Burley, Gerard J. Kleywegt, Haruki Nakamura, John Markley, Jasmine Young, Huanwang Yang, John Westbrook, Sameer Velankar, Sanchayita Sen, Monica Sekharan, Raul Sala, Martha Quesada, Ezra Peisach, Tom Oldfield, Catherine Lawson, Vladimir Guranović, Swanand Gore, Zukang Feng.

**S57**

Total Scattering Pair Distribution Function for Probing Local Structuring and Recrystallization of Amorphous Molecules: A Study of Lactose. Paul Krolikowski, Maxwell W. Terban, Simon Billinge, Steve Hollis, Paul Krolikowski, Eugene Cheung.

**S58**

Two Isomorphic Crystal Structures of Arp2/3 Complex Give Structural Information About Arp2 and Potential N-WASP Binding Sites.

## Posters-S

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Christopher T. Jurgenson, Thomas Pollard,  
Austin Henderson.

### S59

The Structure of a Prophenoloxidase From a Mosquito, *Anopheles Gambiae* Provide New Insights Into the Mechanism of PPO Activation. Yingxia Hu, J. Deng, Y. Wang, H. Jiang.

### S60

X-ray Crystal Structures of Acetylated Lysine Residues in Human Carbonic Anhydrase. Carrie L. Lomelino, Robert McKenna, Melissa Pinard, Jenna M. Driscoll, Antonieta Salguero, Brian P. Mahon.




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## Monday Posters

- M01**  
An Efficient Synthesis, Crystal Structure Determination and Biological Activity of Some Novel Esters Carrying Benzofuran Moiety. C. S. Chidan Kumar, Siddegowda Chandraju, Ching Kheng Quah, Hoong-Kun Fun.
- M02**  
New Insights into Allosteric Regulation of Pyruvate Carboxylase from the structure of the *Aspergillus nidulans* Enzyme. Adam D. Lietzan, Martin St. Maurice.
- M03**  
Superstructure Formation in  $GdFe_xSi_2$  ( $x \sim 0.7$ ): Scaffolding as a Design Principle in Intermetallics. Anastasiya Vinokur, Daniel C. Fredricks.
- M04**  
Structural Basis of Stability of Lig domains Provides a Rationale for Improved Vaccines. Akif Mohd.
- M05**  
Structural Elucidation of the Binding of the Vav-SH2 Domain to the EphA2 Cytoplasmic Region. Kaibo Zhang.
- M06**  
A Blurring of the Distinction Between Disorder and Allo Twinning. Alan D. Rae, Anthony C. Willis, Martin G. Banwell, Ehab S. Taher.
- M07**  
Potential Inhibitors Involved in Glioma. Ketu Bardhi, Paul A. Craig, Herbert J. Bernstein, Kostandina Bard.
- M08**  
 $I_7^-$ : From Stoichiometry to Structural Unit. Alexander J. Blake, Martin Schroder, Amy E. Lisle, Jeremiah P. Tidey.
- M09**  
Alexandrite Effects and Pseudosymmetry in Aluminum Oxalates. Arunpacha Nimthong.
- M10**  
Single Crystal Growth of  $Ca_{12}Al_{14}O_{33}$  - Mayenite. Claudia Rawn, John Salasin, Elijah Barlow.
- M11**  
Cloning, Recombinant Expression and Crystallization of Proliferating Cell Nuclear Antigen from radioresistant archaeon *Thermococcus gammatolerans*. Alberto A. Venancio-Landeros, Enrique Rudiño-Piñera, Cesar Salvador Cardona-Felix.
- M12**  
Systematic Multi-Crystal Data Collection and Processing in JBlufce. Sudhir Babu Pothineni, Robert F. Fischetti, Janet L. Smith, Michael Becker, Ruslan Sanishvili, Sergey Stepanov, Mark C. Hilgart, Craig M. Ogata, Nagarajan Venugopalan.
- M13**  
Study of the Natural Growth Desert Rose Formations, in Particular from the Desert of Chihuahua, a Structural and Chemical Behavior Analysis. Andres Jose Encerrado Manriquez, Alex D. Price.
- M14**  
Temperature and Cooling Rate as Crystallographic Variables. David Moreau, Robert E. Thorne, Jesse Hopkins, Hakan Atakisi.
- M15**  
Mechanical Force Induced Single-Crystal-to-Single-Crystal Phase Transition in Cocrystal  $CuQ2$ -TCNQ. Guangfeng Liu, Yang Liu, Jie Liu, Xutang Tao.
- M16**  
SONICC Sensitivity for Protein Crystal Detection Increased by 5x Utilizing Dye Staining or Labeling. Ellen Gualtieri, Timm Maier.
- M18**  
Non-covalent Interactions Within Complexes Containing Trimeric Perfluoro-ortho-phenylmercury. Eric Reinheimer, Steven Fisher, Ryan Groeneman.

- M19**  
Phenix-Amber: Integrated Molecular Mechanics for Improved Crystallographic Refinement. Pawel A. Janowski, Paul Adams, David Case, Nigel Moriarty.
- M20**  
Using Template-Directed Co-Crystallization to Facilitate Dynamic Molecular Motion and Thermal Expansion in the Organic Solid State. Eric Reinheimer, Leonard MacGillivray, Kristin Hutchins, Ryan Groeneman.
- M21**  
Experimental Strategies for Functional Annotation and Metabolism Discovery: Targeted Screening of Solute Binding Proteins and Unbiased Panning of Metabolomes. Matthew W. Vetting, Nawar Al-Obaidi, Suwen Zhao, Brian SanFrancisco, Jungwook Kim, Daniel J. Wichelecki, Jason T. Bouvier, Hoan Vu, Xinshuai Zhang, Rodionov Dmitry, James Love, Brandan S. Hillerich, Ronald D. Seidel, Ronald J. Quinn, Andrei L. Osterman, John E. Cronan, Matthew P. Jacobson, John A. Gerlt, Steven C. Al.
- M22**  
Chiral BODIPYs. Frank R. Fronczek, M. Graca H. Vicente, Kevin M. Smith, Alex L. Nguyen.
- M23**  
Doping Effects on Thymine Monohydrate Crystals. Elizabeth S. Koch, Jennifer A. Swift, Kelly McKenna.
- M24**  
Structures of the Middle East Respiratory Syndrome Coronavirus 3C-Like Protease, an Anti-Viral Drug Target. George Lountos, David S. Waugh, Danielle Needle.
- M25**  
Synthesis and Characterization of a Bismuth (III)-Organic Hybrid Material. Alyssa K. Adcock, Karah E. Knope.
- M26**  
Structural Details of the OxyR Peroxide-sensing Mechanism. Inseong Jo, Nam-Chul Ha, You-Hee Cho, Soo-Hui Na, Jinsook Ahn, Saemee Song, Jin-Sik Kim, In-Young Chung.
- M27**  
Rapid Experimental SAD Phasing and Hot-spot Identification with a Halogenated Fragment. Joseph D. Bauman, Eddy Arnold, Jerry Joe Harrison.
- M28**  
Characterization of Dihydroorotase from *Methanococcus jannaschii*. Jacqueline Vitali, Michael Colaneri, Aditya Singh.
- M29**  
The Structural Beauty of Nanoparticles. The so far Largest Crystal Structure of a Gold Nanoparticle:  $\text{Au}_{133}(\text{SC}_6\text{H}_4\text{tBu})_{52}$ . Kristin Kirschbaum, Rongchao Jin, Matthew Y. Sfeir, Kannatassen Appavoo, Yuxiang Chen, Chenjie Zeng.
- M30**  
Safer Insecticides: Structure-guided Drug Design Based from Chimeric AChBPs. Janet Bobango, Todd T. Talley, Skylar Wensel, Cassie Huckabay.
- M31**  
A Phenomenon of Co-Crystallization of Diastereomers of Cyanoximes and their Metal Complexes. Nikolay N. Gerasimchuk, Ilia Guzei.
- M32**  
Breaking Barriers in RNA Structural Biology using Serial Femtosecond X-ray Crystallography. Jason R. Stagno, Yun-Xing Wang, John Spence, Petra Fromme, Xinhua Ji, Henry Chapman, Anton Barty, Uwe Weierstall, Thomas White, Garrett Nelson, Ganesh Subramanian, Ping Yu, Nadia Zatsepin, Yuba Bhandari, Chelsie Conrad, Yu Liu, Derek Wendel.
- M33**

Investigation of Polymorphs and Solid-State Phase Transition in Cocrystal: CuQ2-TCNB and PdQ2-TCNQ. Jie Liu, Xutang Tao, Guangfeng Liu.

**M34**

Structural Basis for the Potency and Selectivity of the GSK-3 $\beta$  Inhibitor PF-367. Jeanne Chang, Ravi Kurumbail, Ye Che, Mark Ammirati, Matthew Griffor.

**M35**

Dynamic Reaction Pathways in the Single-Crystal-to-Single-Crystal Solid-State Diels-Alder Reaction of *N,N'*-bis(cyclobutylimino)-1,4-dithiin with 9-Vinylanthracene. Sanaz Khorasani, Demetrius C. Levendis, Manuel A. Fernandes.

**M36**

A Crystallographic Detective Story: Elucidation of the Oxetanocin Biosynthetic Pathway. Jennifer Bridwell-Rabb, Catherine L. Drennan, Hung-wen Liu, Aoshu Zhong.

**M37**

PDBe - Bringing Structure to Biology. Sameer Velankar, Gerard Kleywegt, Michael Wainwright, Robert Slowley, Sanchayita Sen, Eduardo Sanz-Garcia, Gaurav Sahni.

**M38**

Crystal Structure of  $\beta$ -N-acetylglucosaminidase CbsA from *Thermotoga neapolitana*. Jinsook Ahn, Nam-Chul Ha, Inseong Jo, Soo-Hui Na.

**M39**

Novel Uranyl(VI) Complexes Incorporating Propylene-bridged Salen-type N2O2-ligands: A Structural Approach. Saud I. Al-Resayes, Mohammad Azam.

**M40**

An Investigation of the Electron Density of a Jahn-Teller Distorted Cr(II) Cation. John Bacsa.

**M41**

Ribosomal Informatics, Ribosomal Protein

S21. Kevin M. Gibas, William L. Duax, Jocelyn Redlinski, Connor Hu.

**M42**

Crystal Structures and RNA Binding of Two Hfq Homologs from *Aquifex aeolicus*. Kimberley Stanek, Cameron Mura, Jennifer Patterson, Peter Randolph.

**M43**

Potential Application of Expand-Maximize-Compress (EMC) Algorithm on Synchrotron-Based Serial Crystallography. Ti-Yen Lan, Sol Gruner, Veit Elser, Hugh Philipp, Mark Tate, Jennifer Wierman.

**M44**

X-ray Diffraction, Raman, and IR Spectroscopy as Probes for Quantifying Supramolecular Assembly in the Uranyl Solid State. Korey Carter, Christopher Cahill.

**M45**

Structural Basis of *E. coli* dGTPase Hydrolysis and Inhibition Mechanism. Ying Wu.

**M46**

The Small-Angle X-Ray Scattering Core Facility of Center for Cancer Research of National Cancer Institute. Lixin Fan, Yun-Xing Wang, Xianyang Fang.

**M47**

Synthesis and Characterization of New Resveratrol Cocrystals with Improved Physicochemical Properties. Zheng-Zheng Zhou, Ying Zheng, Changquan Calvin Sun, Wei-Jhe Sun, Henry. H. Y. Tong, Wan-Ying Li.

**M48**

Serial Crystallography at FELs - Past Development, Current Capabilities and Future Possibilities. Marc Messerschmidt, Adrian P. Mancuso.

**M49**

GISAXS Pipelines and Analysis. Alexander Hexemer, Sherry Li, Elaine Chan, Singanallur Venkatakrishnan, Abhinav Sarje, Dinesh Kumar.

## Posters-M

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- M50**  
Ionic Liquids as Macromolecule Crystallization Additives. Marc L. Pusey, Joseph Ng, Qunying Yuan, Jorge Barcena.
- M51**  
The Crystal Structure of Entrapped 8-Hydroxyquinoline Molecules in an Interleaved Hydrogen Bonded Zigzag Channel of Sulfamethoxazole Molecules. Emmanuel K. Owusu-Marfo, Amber L. Thompson.
- M52**  
Fragment Screening and Structural Studies of the Transcriptional Cofactor VP30 from Ebola. Matthew C. Clifton.
- M53**  
The Role of PDB-NMA in Crystallography. Monique Tirion.
- M54**  
Recent Update on the Long-wavelength MX Beamline BL-1A at the Photon Factory. Naohiro Matsugaki, Toshiya Senda, Miki Senda, Masahiko Hiraki, Yusuke Yamada, Dorothee C. Lieschner.
- M55**  
C-H Activating Carboxylation of Terminal Alkynes with CO<sub>2</sub> using Copper(I) Complexes. Nigam P. Rath, Abhinav Kumar, Gurmeet Singh, Manoj Trivedi.
- M56**  
Use of High Brilliance, Low Background SAXS Camera for Studies of Macromolecular Solutions. Sergio Rodrigues, Manuel Fernandez-Martinez, Sandra Desvergne-Bléneau, Pierre Panine.
- M57**  
Synthesis, Crystal Growth, and Structural Characterization of Novel Zintl Phases of As, Sb and Bi. Svilen Bobev.
- M58**  
A Synchrotron Light Source for Africa (the AfLS). Tabbetha Dobbins, Guebre Tessema, Herman Winick.
- M59**  
New Developments at the Biological Small Angle X-ray Scattering Facility BL4-2 at SSRL. Thomas Weiss, Lester Carter, Ping Liu, Tsutomu Matsui.
- M60**  
Lipid-directed Cytoskeletal Protein Oligomerization at Sites of Cell Adhesion. Tina Izard.

## Tuesday Posters

### T01

14 years of Neutron Crystallography at the Protein Crystallography Station (PCS). Julian Chen, Clifford Unkefer, John Bacik.

### T02

A Novel Cyclization Mechanism to Biologically Produce Pharmacological Cyclic Compounds: The Crystal Structure of a Terpenoid Cyclase Derived From Short Chains Dehydrogenase/Reductases. Sheng Ye, Rongguang Zhang, Yun Zhu, Lili Qin.

### T03

Active Site Binding Flexibility is Demonstrated by Multiple Structures of the Same Crystal Form of Porphobilinogen Synthase. Ursula D. Ramirez, Eileen K. Jaffe, Trevor Selwood, Linda Stith.

### T04

Anything But Isomorphism: Molecular Symmetry vs. Crystallographic Symmetry in Some Isomeric Trifluoromethyl-Substituted bis-Benzylideneanilines. William H. Ojala, Sarah N. Larson, Anthony L. Gerten, Aaron P. Monson.

### T05

BioSAXS-2000 Advances for Biological Solution Scattering in the Home Laboratory. Mark Del Campo.

### T06

Bridging the Length Scales: Tools to Span the Information Before the Bragg Peaks and Beyond. Katharine Page, Daniel Olds, Hsiu-Wen Wang.

### T07

CCP4 Web Services. Ville Uski, Pavol Skubák, Navraj S. Pannu, Jens Thomas, Fei Long, Marcin Wojdyr, David Waterman, Andrey Lebedev, Eugene Krissinel, Ronan Keegan, Charles Ballard.

### T08

Checking Intensity Corrections on a CCD Detector with a Fiber-optic Taper. Randy Alkire, Frank J. Rotella, Bruce M. Foxman, Aaron R. Gell, Onkei Tai, Shai R. Posner, Anthony H. Nguyen, Logan C. Lorson.

### T09

Co-crystal Structure F Tubulin with PF-06380101, A Novel Auristatin Analogue With Improved Cell. Allison Varghese, Kevin Parris, Jayvardhan Pandit, Suman Shanker, Cynthia Song, Andreas Mader.

### T10

X-ray Structural Determination of a Seleno Carbohydrate-protein Complex with SAD/MAD Phasing. Ryuichi Kato, H. Makyio, T. Suzuki, J. Shimabukuro, M. Kiso, H. Ando, S. Wakatsuki.

### T11

Construction and Structural Determination of a Self-Assembling DNA Macromolecular Crystal. Chad Simmons, Hao Yan, Nadrian Seeman, Yan Liu, Jens J. Birktoft, Fei Zhang.

### T12

Crystal Structure of an Unusual Periplasmic Zinc Binding Protein from *Paracoccus denitrificans*. Erik T. Yukl.

### T13

Crystalline Hydrates: From Two Waters to None without Stopping at One. Milagros Tomas, Rafael Piñol, Larry R. Falvello, Rocío González Álvarez.

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### Flexibility in materials science: the SAXSpace XL nanostructure analyzer

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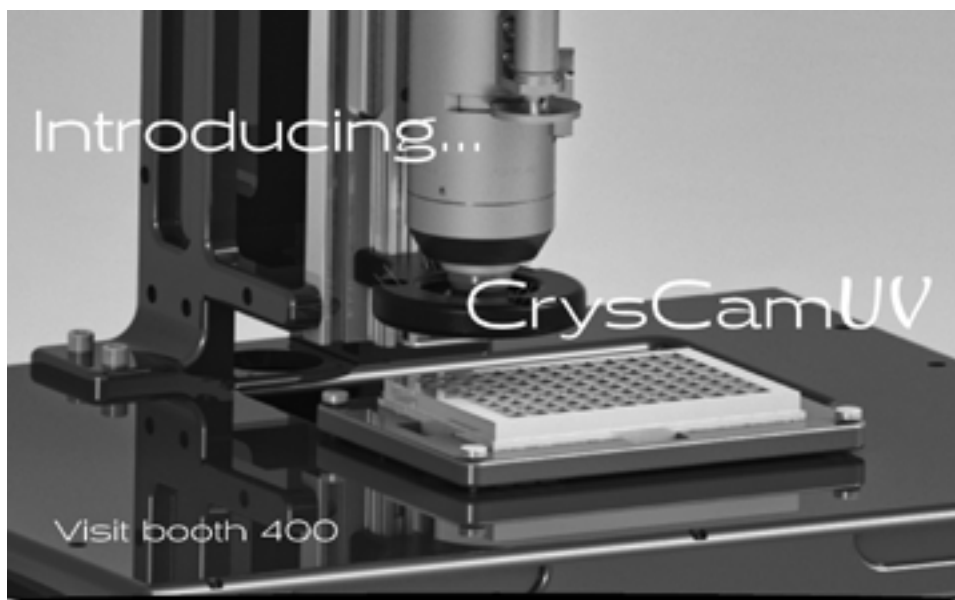
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# Structural Dynamics

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**Ultrafast structural and electronic dynamics of the metallic phase in a layered manganite**

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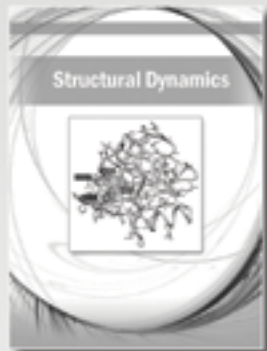
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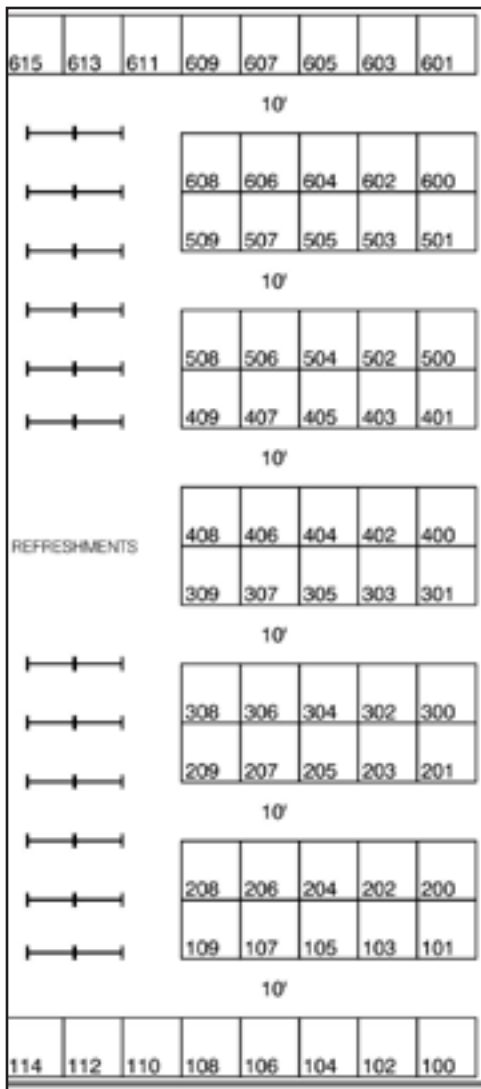
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# 2015 Exhibit Show Liberty Ballroom

**Saturday - 7:30pm - 10:30pm**  
**Sunday, Monday, Tuesday - 10:00am - 7:30pm**

AIP Publishing/Structural Dynamics	#605
American Crystallographic Assn.	#601
American Institute of Physics	#605
Anatrace	#204
Anton Paar	#307
Art Robbins Instruments	#400, 402
Bruker	#500-503
CCDC	#607
CCP4	#209
Continuing Education/USNCCr	#606
Cryo Industries of America Inc.	#509
Douglas Instruments Ltd	#404
Excillum AB	#300
Formulatrix	#401, 403
Huber Diffraction USA	#507
International Center for Diffraction Data	#504
International Union of Crystallography	#302
JAN Scientific, Inc.	#209
Lawrence Berkeley Lab – ALS	#604
MacCHESS/Cornell Univ.	#611
MiTeGen, LLC	#407, 409, 508, 506
Molecular Dimensions Inc.	#200
NatX-ray	#305
Oxford Cryosystems Inc..	#202
Powers Scientific	#405
Rayonix	#309, 408
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Rigaku/Oxford Diffraction	#200, 201, 202, 203
SER-CAT	#609
STOE & Cie GmbH	#306
Structural Dynamics	#603
TA Instruments	#505
TTP LabTech Ltd.	#301, 303
XENOCS SA	#308
XtalConcepts GmbH	#206





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Powder Diffraction .....	Craig Brown
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### About the ACA

The American Crystallographic Association, Inc. (ACA) was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). The objective of ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction. They will also promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from them.

Membership in ACA is open to any person who is actively interested in the purposes of the association and whose application is approved by the ACA Council or its designee. All members are entitled to voting privileges. Student members are very welcome and their contributions to the life and vigor of the association has always been important. The benefits of membership are the same in all categories. These include: voting privileges, RefleXions, the ACA newsletter that is published 4 times per year; complimentary subscription to the Newsletter of the International Union of Crystallography, and Physics Today, a monthly publication of AIP, and reduced rates for the International Tables for X-Ray Crystallography, Structure Reports, Journal of Applied Crystallography, and Acta Crystallographica when purchased for the member's personal use only. ACA is a member society of the American Institute of Physics (AIP) and an Affiliate Member of the International Union of Crystallography.

The total international membership of ACA is about 1,600 with meetings held annually. There are 12 Scien-

tific Interest Groups (SIGs) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Light Sources, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, and Young Scientists. A special division for members residing in Canada is also active. Members may join as many of these groups that are of interest to them. Each SIG is responsible for organizing sessions at Annual Meetings at least every other year.

The headquarters of the association is located at Hauptman Woodward Medical Research Institute, 700 Elicott St., Buffalo, NY 14203.

## MARK YOUR CALENDAR

### Future ACA Meetings:

2016

Denver, Colorado

Friday July 22 - Tuesday July 26

2017

New Orleans, Louisiana

Friday May 26 - Tuesday May 30

2018

Toronto, Ontario, Canada

Friday July 20 - Tuesday July 24

# Program at a Glance

## Morning

WK.02 Serial Crystallography Data Analysis with Cheetah and CrystFEL  
 WK.03 Rietveld Refinement/Analysis  
 WK.04 Small Angle Scattering: Structural Biology and Soft Matter

P1 Warren Award Presentation & Lecture-Laurence Marks  
 1.1.1 Crystallography of Emergent Phenomena I  
 1.1.2 Poster Preview  
 1.1.3 Application of SANS/SAXS to Structural Biology  
 1.1.4 Structural Informatics for Drug D& D  
 T1 Transactions: Crystallography for Sustainability

P2 Burger Award Presentation & Lecture Greg Petsko  
 2.1.1 Porous Materials at the Nano and Meso-scale  
 2.1.2 Crystal Engineering Form & Function  
 2.1.3 General Interest  
 2.1.5 Structural Dynamics  
 2.1.4 Publication Practices

P3 Etter Early Career Award - Yan, Jessie Zhang  
 3.1.1 Etter Early Career Symposium  
 3.1.2 Local Structure and Complex Materials  
 3.1.3 Hot Structures I - Intracellular Protein Regulons  
 3.1.4 Standard Practices in Crystallography I: Data Collection Strategies  
 3.1.5 Structural Modeling for SAS

P4 Plenary Lecture: Juan Manuel Garcia-Ruiz  
 4.1.1 Structural Glycobiology  
 4.1.2 General Interest II  
 4.1.3 In the Service of Science: Experiences and Opportunities with Central Facility Services  
 4.1.4 Important Science from Small Molecular Structures Part II  
 4.1.5 (Bio)Chemistry in the X-ray Beam

Salon 3/4  
 Salon 5/6  
 Philadelphia

Freedom  
 Philadelphia North  
 Philadelphia South  
 Freedom  
 Independence CD  
 Independence AB

Freedom  
 Philadelphia North  
 Philadelphia South  
 Independence CD  
 Freedom  
 Independence AB

Philadelphia South  
 Philadelphia South  
 Independence AB  
 Freedom  
 Independence CD  
 Philadelphia North

Freedom  
 Freedom  
 Independence CD  
 Philadelphia North  
 Philadelphia South  
 Independence AB

WK.02 Serial Crystallography Data Analysis with Cheetah and CrystFEL  
 WK.03 Rietveld Refinement/Analysis  
 WK.04 Small Angle Scattering: Structural Biology and Soft Matter

Student Reception  
**Rigaku Lunch & Learn** 12:00PM  
 1.2.1 From Fingerprinting to Full ID: PXRD  
 1.2.2 Engaging Undergraduates with Crystallographic Research  
 1.2.3 Molecular Machines  
 1.2.4 Biological Macromolecules  
 1.3.1 Career Odyssey

2.2.1 Advances in Multi-crystal Approaches and Serial Crystallography  
 2.2.2 Materials Discovery and Crystal Growth  
 2.2.3 How I Spent my Summer Vacation: Experiences Derived from Small Molecule Summer School  
 2.2.4 SAS with Membranes and Membrane Proteins  
 2.2.5 Mechanistic & Spectroscopic Structural Enzymology  
 2.3.1 Professional Development: Communicating Your Science

3.2.1 Important Science from Small Molecule Structures  
 3.2.2 Powder Pair Distribution Function and Pharmaceuticals  
 3.2.3 Hot Structures from Membrane Systems  
 3.2.4 Standard Practices in Crystallography II: Data Collection Strategies  
 3.2.5 Evolving Techniques for SAS

**Movie: "The Mystery of the Giant Crystals"**  
 4.2.1 General Interest III  
 4.2.2 Cool Structures  
 4.2.3 Structured Nucleic Acids  
 4.2.4 Imaging with X-rays and Electrons  
 4.2.5 Play It Cool? Ambient & Cryogenic Approaches

Salon 3/4  
 Salon 5/6  
 Philadelphia

Philadelphia South  
**Horizons Ballroom**  
 Philadelphia North  
 Freedom  
 Philadelphia South  
 Independence CD  
 Philadelphia South

Independence AB  
 Independence CD  
 Freedom  
 Philadelphia North  
 Philadelphia South  
 Philadelphia South

Philadelphia South  
 Independence AB  
 Freedom  
 Independence CD  
 Philadelphia North

**Independence AB**  
 Independence CD  
 Philadelphia South  
 Freedom  
 Independence AB  
 Philadelphia North

## Evening

**Student Orientation**  
 Opening Reception/Exhibit Show

Salon 10  
 Liberty Ballroom

**Poster Session 5**  
 sponsored by Art Robbins Instruments  
**Breaker-YSSIG Mixer**

05:30pm  
 08:00pm  
 12:00pm  
 12:00pm  
 05:00pm

**Poster Session M**  
 2.3.2 Would You Publish This?

Philadelphia North  
 Philadelphia North  
 Philadelphia North  
 Philadelphia South  
 Independence AB  
 Independence AB

3.3.1 Evening Session on Diversity  
**Poster Session T**  
 Business Meeting for all  
 ACA Members

Freedom  
**Liberty Ballroom**  
 Philadelphia North  
 Philadelphia North  
 Philadelphia North  
 Freedom  
 Independence CD

**SIG MEETINGS**  
 Small Angle Scattering  
 BioMac SIG Meeting  
 Joint: Small Molecules & Service

12:00pm  
 12:00pm  
 12:00pm

**Annual Awards Banquet**  
 (ticket required)  
 Cash Bar 6:30pm  
 Dinner 7:30pm

**Liberty Ballroom**

## 2015 EXHIBIT SHOW

Liberty Ballroom

**Saturday, 7:30pm-10:30pm**    **Sunday, Monday, Tuesday, 10:00am-7:30pm**

Saturday  
 July 25

Sunday  
 July 26

Monday  
 July 27

Tuesday  
 July 28

Wednesday  
 July 29

Thursday  
 July 30

Planning Session for 2016 Meeting in Denver  
 8:30am

Horizons Ballroom