Annual Meeting  May 26 - 30, 2017

Program Chairs:  Yulia Sevryugina & Ilia Guzei

Poster Chair:  Bruce Noll

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- Rayonix
WK.01 CSD Workshop
Communication and Innovation
Organizers:  Strand 12
Pete Wood (CCDC, UK)
Suzanna Ward (CCDC, UK)
Andrew Maloney (CCDC, UK)

This workshop, split into two sessions, is focused on the Cambridge Structural Database (CSD), the world’s repository for all small molecule organic and metal-organic crystal structures, and it’s associated suite of software tools. The morning session (Part A: Communication and Education) will highlight how free services available through CSD-Community can exploit the knowledge contained in the CSD to aid both education and research. The afternoon session (Part B: Advanced Research Applications) will take attendees through a range of fundamental, intermediate and advanced research applications of the CSD Python API.

WK.02 CryAlis and OLEX2: From Raw Data to Publication
Organizers:  Celestin A
Eric Reinheimer, Carla Slebodnick, Charlotte Stern

This workshop will provide software training with the freely available programs CrysAlisPro and Olex2, covering the complete small molecule crystallography workflow—from processing the raw images through uploading the final CIF to checkCIF. The workshop format will include brief background lectures followed by hands-on practical sessions. The morning sessions will focus on the theoretical and practical aspects of data processing using CrysAlisPro. Topics will include data processing of single and twinned crystals, absorption corrections and scaling, and publication. The afternoon session will focus on the Olex2 graphics program for structure solution and refinement. Two datasets will be drawn from the morning session and will include a routine sample and a complex samples that highlights the powerful disorder modeling features in Olex2. The participants will also leave with hands-on experience using more advanced features of both programs. Documentation will be provided so participants can transfer their new-found knowledge to their home institutions.
WK.03 Introduction to PHENIX for Beginning and Advanced Crystallographers
Chair: Celestin B Paul Adams

The purpose of the workshop is to train both beginning and advanced crystallographers in the use of the PHENIX software for macromolecular structure determination. The workshop will benefit the crystallographic community by making the use of this software accessible to a broader group of crystallographers, by teaching crystallographers when and how to use the software properly, and by teaching crystallographers how to get the most out of the software.

The workshop will have two components. The morning session will introduce the PHENIX system and the core algorithms that it uses. The afternoon session will be a hands-on tutorial for beginning and intermediate users concurrent with individual tutorials for advanced users.

The morning session will begin with an overview of PHENIX that introduces what the PHENIX software can do, how it is organized, and how it is used. Then the core automation in PHENIX will be presented along with the key algorithms used in structure solution by MIR/MAD/SAD, molecular replacement, density modification and automated model-building. Next the algorithms for structure refinement will be described with emphasis on the core concepts. Then the extensive validation available during and after structure determination with PHENIX will be described. Finally the attendees will learn how to use the GUI to carry out all the methods used in PHENIX.

In the afternoon there will be three group tutorials. The first will focus on data analysis (twinning, space groups, structure factor statistics) and structure solution (finding an anomalous substructure in a MAD or SAD dataset). The second tutorial will focus on molecular replacement, model-building and ligand fitting. The third will cover refinement and validation. Concurrent with the tutorials, advanced users will have individual tutorials on their own data.

08:30 PHENIX Overview. Paul Adams
08:45 Automation of Structure Determination. Tom Terwilliger
09:30 Molecular Replacement. Paul Adams
10:00 Coffee Break and set-up of PHENIX on individual computers
10:30 Refinement in PHENIX. Pavel Afonine
11:15 Model Validation. Paul Adams
11:45 The PHENIX GUI. Billy Poon
12:15 Discussion
12.30 Lunch
1:30-4:30 Individual tutorials for advanced users and group tutorials for beginning and intermediate users
1:30PM-2:30 Hands-on Tutorial - Data analysis and Structure solution
2:30-3:30 Hands-on Tutorial - Molecular Replacement, Model-building and Ligand Fitting
3:30-4:30 Hands-on Tutorial - PHENIX Refinement and Validation
4:30 Workshop Survey and wrap-up
FRIDAY, MAY 26

WK.04 Research Data Management

Chairs: Celestin C John Helliwell, Brian McMahon, Tom Terwilliger

This workshop focuses on essential elements of research data management for the practising crystallographer. The morning session explores what every experimentalist needs to know about recording essential metadata of primary (i.e. raw) diffraction data; the afternoon session considers elements of research data management policy mandates and requirements on Principal Investigators (PIs), including metadata standardisation, data repositories, and primary data linking to publications.

08:30-08:40

08:40-09:00
The Science International Accord on Open Data in a Big Data World and the IUCr’s response. Marvin Hackert, Brian McMahon, Luc Van Meervelt, John Helliwell.

09:00-09:30
What Every Experimentalist Needs to Know about Recording Essential Metadata of Primary (i.e. Raw) Diffraction Data. Herbert J. Bernstein.

09:30-10:00

10:30-11:00
Research Data Management at CHESS. D. Marian Szebenyi, Devin Bougie, Aaron Finke, Richard Gillilan, Jesse Hopkins, David Schuler and Werner Sun.

11:00-11:30

13:00-13:30
Open Science and Research Data policy mandates and requirements on Principal Investigators (PIs). Simon Hodson.

13:30-14:00

14:00-14:30

14:30-15:00
Research Data Management: administration, raw diffraction data, structure factors and coordinates at the UK’s National Crystallographic Service (NCS). Simon Coles.

15:00-15:30
SBGrid Databank. Peter Meyer, Jason Key, Merce Crosas and Piotr Sliz.

15:30-16:00
General discussion on research data management policy mandates and requirements

WK.04-II

16:15-16:45

16:45-17:15
Intel Scalable System Framework. Henry Gabb.

17:15-17:45
Intel Software and Programming Tools Ecosystem for HPC. Henry Gabb.

17:45-18:15
General discussion on high-data-rate/high-performance-computing issues of research data management for MX
Friday Evening Activities

First Time Attendee and Student Meeting Orientation
05:30-06:30pm  Strand 12  (2nd floor)
The focus of this informal session is to orient young scientists and first time attendees to the structure of our meeting and how to make the most of their experience.

Special Plenary Lecture
06:30-7:30pm  Celestin A
Sir James Fraser Stoddart, 2016 Nobel Laureate in Chemistry
“How Crystallography Helped to Create the Mechanical Bond in Chemistry”

Opening Reception and Exhibit Show
07:30pm  Storyville Hall
Must have meeting name badge for entry
## P1.1 Poster Preview

**Chair:**  
Celestin A  

**Bill Duax**

**07:45-07:51**  

**07:51-07:57**  
Identification of Lead Compounds for Inhibitor Design against Tyrosyl DNA Phosphodiesterase I by Crystallographic Fragment Screening. George Lountos, Xue Zhi Zhao, Evgeny Kiselev, Joseph Tropea, Danielle Needle, Terrence Burke, Yves Pommier and David Waugh.

**07:57-08:03**  
Evolutionary conservation of structure and function in the plant aldehyde dehydrogenase 12 family. David A. Korasick, John J. Tanner.

**08:03-08:09**  

**08:09-08:15**  
Structural evolution and substrate specificity of Family GH31 α-glucosidases and their contribution to starch digestion. Marcia Chaudet, David Rose and Kyra Jones.

**08:15-08:21**  
A Structural Study of Quinolinate Synthase, a Key Enzyme in Bacterial NAD+ Biosynthesis. Neela Yennawar, Olga Esakova, Tyler Grove, Alexey Silakov, Allison Saunders, Martin McLaughlin and Squire Booker.

**08:21-08:27**  

**08:27-08:33**  
Induced fit in the specific recognition of transition metal ions by a gene-regulatory RNA. Sharrol Bachas, Adrian Ferre-D’Amare.

**08:33-08:45**  
Crystal structures and small angle x-ray scattering analysis of antifungal drug target aspartate semialdehyde dehydrogenase. Gopal Dahal, Shuo Qian and Ronald Viola.

**08:39-08:45**  
Trapping conformational states of the SidA ornithine hydroxylase in crystallo. Ashley Campbell, John Tanner, Ritcha Mehra-Chaudhary, Julia Del Campo, Pablo Sobrado.

## P1.2 Poster Preview

**Chair:**  
Celestin C  

**Daniel Mast**

**07:45-07:51**  

**08:27-08:33**  
Induced fit in the specific recognition of transition metal ions by a gene-regulatory RNA. Sharrol Bachas, Adrian Ferre-D’Amare.

**08:33-08:45**  
Crystal structures and small angle x-ray scattering analysis of antifungal drug target aspartate semialdehyde dehydrogenase. Gopal Dahal, Shuo Qian and Ronald Viola.

**08:39-08:45**  
Trapping conformational states of the SidA ornithine hydroxylase in crystallo. Ashley Campbell, John Tanner, Ritcha Mehra-Chaudhary, Julia Del Campo, Pablo Sobrado.
08:03-08:09

08:09-08:15

08:15-08:21
Hard X-ray-Induced Valence Tautomeric Interconversion in Cobalt-o-Dioxolene Complexes. Carlos Pinheiro.

08:21-08:27

08:27-08:33
Phase retrieval algorithms for direct phasing of coherent nanocrystal diffraction. Joe Chen and Richard Kirian.

08:33-08:39
Structural Investigation of a Novel Sulfonamide Chalcone Hybrid. Lidiane J. Michelini.

09:00-09:20
Perspectives on the cryo-EM - Resolution Revolution from the Protein Data Bank. Stephen Burley.

09:20-10:00
The cryoEM structures of immature and mature Zika virus and of mature Zika virus complexed with a human monoclonal antibody. Michael Rossmann.

10:00-10:30 Coffee Break

10:30-11:10
The power of cryo-electron tomography. Wolfgang Baumeister.

11:10-11:35
CryoEM Structure of Dynamin-like MxB in Assembly. Peijun Zhang, Frances Alvarez, Shaoda He, Juan Perilla, Sooin Jang, Alan Engelman and Sjors Scheres.

11:35-12:00
Near-atomic resolution visualization of human transcription promoter opening. Yuan He.
12:00-12:25
Structural Biology of Bacterial Transcription. Seth Darst, James Chen, Jin Young Kang and Elizabeth Campbell.

12:25-13:30 Lunch Break

13:30-13:55
In situ structures of the genome and genome-delivery apparatus in an ssRNA virus. Hong Zhou, Xinghong Dai, Zhihai Li, Mason Lai, Sara Shu, Yushen Du and Ren Sun.

13:55-14:20
Cryo-EM structure determination of small protein complexes with the Volta phase plate. Maryam Khoshouei, Radostin Danev, Mazdak Radjainia and Wolfgang Baumeister.

14:20-14:45
Atomic resolution structure determination by the cryo-EM method MicroED. Tamir Gonen.

14:45-15:10
4D electron microscopy with a millisecond temporal resolution. Shigeki Watanabe.

15:10-15:30 Coffee Break

15:30-15:55

15:55-16:20
CryoEM of Molecular Machines. Wah Chiu.

16:20-16:50 Speaker Round Table

16:50-17:00

1.1.1 Hybrid Methods - BioSAXS
Session Chairs: Michael Hammel, Greg Hura

09:00-09:20
Contrast matching of detergent micelles for membrane protein studies with SANS. Ryan Oliver.

09:20-09:40
A new method for computational purification of complex mixtures by chromatography-coupled SAXS. Steve Meisburger, Alexander Taylor, Crystal Khan, Shengnan Zhang, Paul Fitzpatrick and Nozomi Ando.

09:40-10:00
Coflow - a step forward for solution SAXS. Nigel Kirby and Tim Ryan.

10:00-10:30 Coffee Break

10:30-10:50
SAXS: A Versatile Tool to Study Biological Macromolecules in Solution. Srinivas Chakravarthy, Thomas Irving, Osman Bilssel and Sagar Kathuria.

10:50-11:10

11:10-11:25
Resolution and validation of SAS-based structural models. Anne Tuukkanen, Gerard J. Kleywegt and Dmitri Svergun.

11:25-11:40
Conformational properties integral to the phase separation properties of hnRNPA1 revealed by small angle X-ray scattering. Erik Martin, Nicole Milkovic and Tanja Mittag.

11:40-12:00
Fc plasticity studies by Small Angle X-
1.1.2 Disorder, Imhomogeneity, and Local Structure in Complex Materials

**Session Chairs:** Celestin B Milinda Abeykoon, Martin Donakowski

09:00-09:20 Characterizing disorder in space and time. Takeshi Egami.


09:40-10:00 Role of Diastereomeric Solid-Solution Disorders in Limiting Resolution for Spatially Similar Enantiomers: Case Studies using Spiroborate Anions. Ian Duncan Williams, Lawrence Wan-Yin Wong, Gemma Shuk-Shan Tam and Herman Ho-Yung Sung.

10:00-10:30 Coffee Break

10:30-10:50 Dynamic local symmetry breaking: the key for understaning devices from energy conversion to superconductivity? Simon Billinge.

10:50-11:10 Chalcogels as electrode materials for Li-ion batteries. Vicky Doan-Nguyen, Kota Subrahmanyam, Megan Butala, Jeffrey Gerbec, Saiful Islam, Katherine Kanipe, Catrina Wilson, Mahalingam Balasubramanian, Kamila Wiaderek, Olaf Borkiewicz, Karen Chapman, Peter Chupas, Martin Moskovits, Bruce Dunn, Mercouri Kanatzidis and Ram Seshadri.

11:10-11:30 X-ray Absorption Spectroscopy with other simulation techniques to work on amorphous and nano-systems. Yuanpeng Zhang.

11:30-11:45 Relating $\Sigma$-LiVOPO$_4$ performance to local environment dynamics and hysteresis. Kamila Wiaderek, Olaf Borkiewicz and Karena Chapman.

11:45-12:00 DISCOVER: ORNL’s Total Scattering Diffractionometer for Materials Discovery. Katherine Page, Matthew Tucker and Patrick Woodward.

1.1.3 Utilization of Small Molecule Crystallography in Pharmaceutical Development

**Session Chairs:** Andrew Brunskill, Milan Gembicky

09:00-09:20 Am I Seeing Double? Absolute Configuration and X-ray Crystallography. Bruce C. Noll, Holger Ott, Michael Ruf and Tobias Stuerzer.

09:20-09:40 Crystal packing and pharmaceutical properties of salts of diclofenac. Carl Schwalbe, Miren Ramirez, Barbara Conway and Peter Timmins.

09:40-10:00 Academic and Industrial Partnerships for the Betterment of All. Curtis Moore and Milan Gembicky.

10:00-10:30 Coffee Break


11:00-11:30 Driving Pharmaceutical Development with Small Molecule Crystallography: Not Just a Pretty Picture. Andrew Brunskill.
11:30-12:00
Applying structural informatics approaches to pharmaceutical supply chain processes. Andrew G. P. Maloney, Mathew J. Bryant and Neil Feeder.

1.1.4 Engaging Undergraduates with Crystallographic Research
Chairs: Celestin E Rachel Powers, Joe Tanski
Funding provided by CCDC, Bruker

09:00-09:20
Teaching Chemical Crystallography Without a Diffractometer. Tim Royappa.

09:20-09:40
3D Chemistry: How 3D printing could help embed crystallography within chemistry undergraduate teaching. Peter Wood, Amy Sarjeant, Ian Bruno, Clare Macrae, Helen Maynard-Casely and Matthew Towler.

09:40-10:00
A taste of crystallographic research for undergraduate students via a problem-based approach. Simon Coles, Peter Horton, Lucy Mapp and Sarah Milsted.

10:00-10:30 Coffee Break

10:30-10:50
Integrating Undergraduate Interns Into an X-ray Diffraction Infrastructure. Richard Matyi.

10:50-11:10
Structures with Interesting and Instructional Features from a Discovery Based Molecular Structure Determination Lab Module for Undergraduates Since 2010. Joseph Tanski.

11:10-11:30
Cooperative Approaches in Introducing Undergraduates to Protein Crystallography. Krystle McLaughlin.

11:30-12:00
From Cloning to Protein Structures: Engaging undergraduates in Protein Structural Biology at Bryn Mawr College. Bradley Miller.

Undergraduate Research Symposium
Chairs: Celestin E Brad Conrad, Krystle McLaughlin

12:00
All undergraduates, graduate students, and their mentors are invited for a reception highlighting undergraduate research. Posters prepared on research of undergraduates will be highlighted and refreshments will be provided.

1.2.1 Nucleic Acids and Friends
Chairs: Celestin A Eric Montemayor, Aaron Robart
Funding provided by ELGA LabWater, USA, Hampton Research Corp., Integrated DNA Technologies, MiTeGen, VWR International Co.

13:30-13:50
Atomic structure of *S. cerevisiae* U1 snRNP offers insight into alternative splicing. Rui Zhao.

13:50-14:10
Structure and Function of a snoRNP Maturation Complex. Hong Li.

14:10-14:30
Crystal structure of the *Rous sarcoma* virus intasome. Hideki Aihara.

14:30-15:00
Ruler-based mechanisms of ribonuclease III enzymes. Xinhua Ji.

15:00-15:30 Coffee Break

15:30-15:50
Atomic structures of kinetoplastid RNA editing sites. Blaine Mooers.
15:50-16:10
Enzymatic Removal of Epigenetic Marks from DNA. Alex Drohat.

16:10-16:30
Mechanism and evolution of the DNA repair enzyme MutY. Martin Horvath, Evan Drage, Emily Dart, Peyton Russellburg, Valerie O’Shea, Ryan Woods, Aurea Chu, Sheng Cao, Jody Richards and Sheila David.

16:30-16:50
Nucleic Acid Crystallization and Phase Determination Facilitated by Selenium Functionalization. Zhen Huang and Xinghua Chen.

1.2.2 Diffuse Scattering in Complex Oxides
Chairs: Celestin B
Ben Frandsen, Katharine Page

13:30-14:00
Cuproirdisite - orbital parts unknown. Emil Bozin.

14:00-14:30
Unraveling atomic motions through Dynamic Pair Distribution Function Analysis. Allyson Fry-Petit.

14:30-15:00
The various contributions to the diffuse scattering from PMN-xPT. Daniel Phelan, Matthew Krogstad, Peter Gehring, Stephan Rosenkranz, Ray Osborn, Zuo-Guang Ye, Feng Ye, Yaohua Liu, Jacob Ruff and Justin Wozniak.

15:00-15:30 Coffee Break

15:30-15:50
Polar nanoregions and single crystal diffuse scattering in relaxor ferroelectrics. Richard Welberry.

15:50-16:10
Revealing the local atomic and magnetic structure of a new dilute ferromagnetic semiconductor by pair distribution function analysis. Benjamin Frandsen.

16:10-16:30

16:30-16:45

16:45-17:00

1.2.3 Advances in Room Temperature Data Collection: Revealing Dynamics and Function
Chairs: Celestin C
Gerd Rosenbaum, Rob Thorne

13:30-14:00

14:00-14:30
Automated room temperature ligand screening on beamline FIP at the ESRF. Jean-Luc Ferrer.

14:30-15:00
First results from the long-wavelength macromolecular crystallography beamline I23 at Diamond Light Source. Armin Wagner, Ramona Duman, Kamel El Omari, Vinay Grama and Vitaliy Mykhaylyk.
15:00-15:30 Coffee Break

15:30-16:00

1.2.4 Important Science from Small Molecules

Chairs: Celestin E Alberto Albinati, Korey Carter

Funding provided by Crystallographic Research, Inc., Dectris

13:30-13:50

13:50-14:20
Intriguing Aspects of Non-innocent Ligands in Transition Metal Complexes. Michael Hall.

14:20-14:40
Synthesis of pyridinium transition metal tetrachlordides counter-ions as starting materials for coordination of organic ligands. Raul Castaneda and Jaclyn Brusso.

14:40-15:00
Rhenium reactivity - manipulation by ligand development. Alice Brink, Hendrik G. Visser and Andreas Roodt.

15:00-15:30 Coffee Break

15:30-15:50
Combining Crystallography and Complementary Techniques to Understanding Small Structural Changes in Intermetallic Compounds and Sulfides. Robin Macaluso.

15:50-16:15
Weak Bonding Interactions, Large Structural Impact. Carlos Murillo.

16:15-16:30

16:30-16:40

16:40-17:00
P2 Patterson Award and Lecture
Amy Sarjeant, Presiding
Celestin D

08:00-08:45am
The Patterson Award for a Lucky Crystallographer. Zbigniew Dauter, Argonne National Lab

SIG MEETINGS
Young Scientist Meeting ....................................................... 12:00pm ............................................................. Celestin D
Neutron, Materials, Powder Joint Meeting ............................ 12:00pm ............................................................. Celestin B
Biological Macromolecules Meeting ...................................... 5:00pm ............................................................. Celestin C

2.1.1 Learn Macromolecular Crystallography; Best Practices with Diffraction Images from a Known X-ray Structure
Chairs: Celestin E
Stephen Burley, Wladek Minor
Funding provided by Anton Paar, Bristol-Myers Squibb, Bruker AXS, Dectris, HKL Research, Janssen Research & Development, Rigaku, Genentech

09:00-09:10
Welcome, Introductions, Session Objectives. S. Burley.

09:10-09:40

09:40-10:00
Introducing the Case Study. Wladek Minor.

10:00-10:30 Coffee Break

10:30-10:55
The science of diffraction data collection. Zbigniew Dauter.

10:55-11:20
SAD phasing for easy or challenging problems. Thomas Terwilliger.

11:20-11:30
Case Study Progress Review. Wladek Minor.

11:30-11:55

11:55-12:20

12:20-12:30
Case Study Conclusion. Wladek Minor.

2.1.2 Joint Methods for High Rate Data Processing: XFEL and Synchrotron
Chair: Celestin D
Herbert Bernstein, Nicholas Sauter

09:00-09:20
Combining new data collection tools and improved beam delivery on the macromolecular crystallography beamline I04 at Diamond Light Source. Ralf Flaig, Pierpaolo Romano, Jonathan Blakes, Chris Bloomer, Graham Duller, Sandira Gayadeen, Michael Hillman, James O’Hea, Geoff Preece, Graeme Winter and David Hall.

09:20-09:40
On Target: Progress in serial crystallography using fixed targets at XFELs and Synchrotrons. Danny Axford, Darren Sherrell and Robin Owen.

09:40-10:00
Synchrotron Serial Crystallography with Multi-stage Merging of 1000’s of Images. Herbert J. Bernstein, Lawrence C.

10:00-10:30 Coffee Break

10:30-10:50
Integration optimization, triage and analysis tools for serial crystallography. Artem Lyubimov.

10:50-11:10
Improving the models for diffraction used in serial crystallographic data reduction. Aaron Brewster.

11:10-11:30
Resolution of the resolution limit. James Holton.

11:30-11:50
High data rate processing - a puzzle of metadata, compression and software. Andreas Foerster.

11:50-12:00
Group Discussion: What gaps remain for serial crystallography data processing? Nicholas Sauter.

2.1.3 Porous Materials

Chairs: Celestin B
Paul Forster, Andrey Yakovenko

09:00-09:30

09:30-10:00
Structural flexibility in the solid state. Len Barbour.

10:00-10:30 Coffee Break

2.1.4 NMR Crystallography

Chairs: Celestin C
Tomislav Friscic, Manish Mehta

Funding provided by Bruker

09:00-09:10 Introduction. Manish Mehta

09:10-09:40

09:40-10:00

10:00-10:30 Coffee Break

2.1.4 NMR Crystallography

Chairs: Celestin C
Tomislav Friscic, Manish Mehta

Funding provided by Bruker

09:00-09:10 Introduction. Manish Mehta

09:10-09:40

09:40-10:00

10:00-10:30 Coffee Break

10:30-11:00

11:00-11:30

11:30-12:00
Metal-organics: A rich seam of data for knowledge mining. Peter Wood.

SUNDAY, 28
11:30-12:00

2.1.5 Cool Structures
Chairs: Celestin A
Jeff Bertke, Richard Staples

09:00-09:20
Engaging the terminal: highlighting routes for promoting non-covalent interactions with uranyl oxo atoms. Korey Carter, Christopher Cahill, Mark Kalaj.

09:20-09:40

09:40-10:00
Alchemy in the 21st Century! Carla Slebodnick, Victoria Soghomonian and Qifan Yuan.

10:00-10:30 Coffee Break

10:30-10:50
Crystalllographic Analysis of Analogous Silicon- and Carbon-Containing Di(Cyanate Ester)s and Tri(Cyanate Ester)s. Kamran Ghiasi, Andrew Guenthner, Sean Ramirez, Michael Ford, Denisse Soto, Jerry Boatz and Joseph Mabry.

10:50-11:10
Selective binding of weakly coordinating anions: exploring the conformational space of flexible receptors. Ivica Dilovic and Krunoslav Uarevic.

11:10-11:25
_in-situ_ reduction study of anion concentration and its effects in the Fe-Ga-S system. Rebecca McAuliffe and Daniel Shoemaker.

11:25-11:40

11:40-12:00
Composition-dependent variations in displacement, occupational and density modulation waves in plagioclase feldspar \([Na_{1-x}Ca_x(Si_{3-x}Al_{1+x}O_8})\] solid solution with incommensurately modulated structure. Huifang Xu and Shiyun Jin.

2.2.1 Enzymes of Post-Translation-al Modifications
Chairs: Celestin C
Bernhard Lechtenberg, Carrie Wilmot

13:30-14:00
Structural Principles of Protein Kinase Regulation. Frank Sicheri.

14:30-15:00
Identifying three-dimensional structures of autophosphorylation complexes in crystals of protein kinases. Roland Dunbrack and Qifang Xu.

14:30-15:00
Characterization of non-active site, TrkA selective kinase inhibitors and implications on obtaining kinase selectivity. Hua Su, Keith Rickert, Christine Burlein, Kartik Narayan, Marina Bukhtiyarova, Danielle Hurzy, Craig Stump, Xufang Zhang, John Reid, Srivanya Tummala, Jennifer Shipman, Steven Carroll, Stephen Soisson, Darrell Henze and Andrew Cooke.

15:00-15:30 Coffee Break

15:30-16:00
Molecular mechanism for the regualtion of yeast separase by securin. Shukun Luo and Liang Tong.

16:00-16:30
Structural insights into bacterial lipoprotein
biosynthesis. Cameron Noland, Michele Kattke, Susan Gloor, Jingyu Diao, Homer Pantua, Sharookh Kapadia and Jeremy Murray.

16:30-17:00

2.2.2 Home-Built Software

Chairs: Larry Falvello, Victor Young

13:30-14:00
Research and teaching tools: A SHELX/POV-Ray interface (X-Seed) and simulation of a diffractometer (SMART1k). Len Barbour.

14:00-14:20

14:20-14:40

14:40-15:00
Using the CSD Python API for interactive analytics and data mining of the Cambridge Structural Database. Paul Sanschagrin.

15:00-15:30 Coffee Break

15:30-16:00
From Special Least-Squares to Twin Laws: My Toolbox of Programs from 1964 to 2017. Bruce Foxman.

16:00-16:20

16:20-16:40

16:40-17:00
What is new in Olex2. Horst Puschmann and Oleg Dolomanov.

Session 2.2.3 General Interest I

Chairs: Madushani Dharmarwardana, Carla Slebodnick

13:30-13:50
Bence-Jones Protein Pav: the first ISIR structure. John Rose and Bi-Cheng Wang.

13:50-14:10
Glycines Job Security Revealed by X-ray crystallography. William Duax.

14:10-14:30

14:30-14:45

14:45-15:00
Amino Acid Physical Chemistry Furnishes a Two-Dimensional Basis Set for Computational Structural Biology. Charles Carter.

15:00-15:30 Coffee Break

15:30-15:50
15:50-16:10
How to Assign a (3+1)D Superspace Group to an Incommensurately Modulated Biological Macromolecular Crystal. Gloria Borgstahl, Jason Porta and Jeffrey Lovelace.

16:10-16:30
Direct observation of protonation states in a PLP-dependent enzyme by neutron crystallography. Andrey Kovalevsky, Steven Dajnowicz, Matthew Blakeley, David Keen and Timothy Mueser.

16:30-16:45

16:45-17:00
Modern, rigorous macromolecular crystallographic refinement using mixed-QM/MM functional methods as implemented in DivCon. Oleg Borbulevych and Lance M Westerhoff.

2.2.4 Integrative Approaches to Structural Biology (NMR, cryoEM, SAS)
Chairs: Celestin E Kushol Gupta, Michael Hammel
Funding provided by Anton Paar USA

13:30-13:50
Super resolution for X-ray scattering and biological insights from its applications to dynamic DNA replication and repair complexes. John Tainer.

13:50-14:10

14:10-14:30
BECN Homologs and ATG14 Form a Conserved, MetastableaCoiled-Coil to Mediate Autophagy. Sangita Sinha, Minfei Su, Yang Mei, Yue Li and Christopher Colbert.

14:30-15:00

15:00-15:30 Coffee Break

15:30-15:50
Crystal structure of the human calpain-5 catalytic core. Gabriel Velez, Vinit Mahajan, Lokesh Gakhar, Saif Khan, Hanna Koster, Jing Yang, Stephen Tsang, Alexander Bassuk.

15:50-16:10
An Integrative Approach to Exploring the Role of Oligomerization in Enzyme Function. John Tanner.

16:10-16:30
Structural Basis of Drug-Induced Aggregation of HIV-Integr. Kushol Gupta.

16:30-17:00
High energy fun, great food and some of the most exciting venues make the 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 Gordon Biersch, 200 Poydras Street, New Orleans, LA 70130. http://www.gordonbiersch.com/locations/new-orleans?action=view
Mixer begins at 8:00pm and is sponsored in part, by Bruker, AXS.

Peter Ercius, Gerardo Martinez, Lewys Jones, Martin Huth, Martin Simson, Heike Soltan, Yukihito Kondo, Ryusuke Sagawa, Timothy Pennycook and Peter Nellist.

16:30-17:00
Probing structural dynamics in charge-density-wave TaSe$_2$, TaTe$_2$ using ultrafast electron diffraction. Jing Tao, Junjie Li and Jun Li.

2.3.1 Diversity and Inclusion

Chairs: Oluwatoyin Asojo, Krystle McLaughlin

18:30-18:50
L@S GANAS: Latin@’s Gaining Access to Networks for Advancement in Science. Bernard Santarsiero.

18:50-19:10
Strategies for developing successful Crystallography Research programs with diverse students. Oluwatoyin Asojo.

19:10-19:30
Diversity and Inclusion - Steady Progress by Degrees. Cheryl Stevens.
3.1.1 Materials for a Sustainable Future

Chairs: Celestin A
Vicky Doan-Nguyen, Kamila Wiaderek

09:00-09:30

09:30-10:00
Crystalline Products of CO₂ Capture by Amines. Tatiana Timofeeva, Victoria Sena, Sofia Antal, Omar Cano, Boris Averkiev.

10:00-10:30 Coffee Break

10:30-11:00
High-valent states in cobalt and nickel oxygen-evolving catalysts and their role in O-O bond formation. Ryan Hadt.

11:00-11:20
On the design and development of ion conducting oxides. Craig Bridges.

11:20-11:40
Weak bonds in an aged cellulose chromaphore precursor by crystallography and computed charge density. Alfred French, Kurt Mereiter and Thomas Rosenau.

11:40-12:00
Li/Ag₂VO₂PO₄ batteries: the roles of composite electrode constituents on electrochemistry. Andrea Bruck, Esther Takeuchi, Amy Marschilok and Kenneth Takeuchi.

3.1.2 Mineralogical Crystallography

Chairs: Aaron Celestian, Nichole Valdez

09:00-09:15
High-pressure single crystal study of dravite. Earl O’Bannon.

09:15-09:30

09:30-09:45
Chemical zoning in minerals. Sytle Antao, Jeffrey Salvador, Laura Cruickshank and Inayat Dhaliwal.

09:45-10:00
Accurate and precise thermal expansivities of kyanite, andalusite and sillimanite, from 10 - 1573 K measured using time-of-flight neutron powder diffraction. A. Dominic Fortes.

10:00-10:30 COFFEE BREAK.

10:30-10:45
The incommensurately modulated structures and ordering sequence of Na-rich plagioclase feldspars. Shiyun Jin, Huifang Xu.

10:45-11:00
Low temperature structural investigations along the Cu₃SbS₃ (skinnerite) - Cu₃BiS₃ (wittichenite) join.. Neil Johnson, Elinor Spen-
3.1.3 Using Standard Tools & Methods in Non-standard Ways
Chairs: Celestin B Milan Gembicky, Andrey Yakovenko

09:00-09:20
Getting the most out of your high pressure experiments! Michael Ruf.

09:20-09:40

09:40-10:00
Approximating the near K-edge mass absorption coefficients of Ni using an ultra-thin bi-metal Ti-Ni foil. Randy Alkire.

10:00-10:30 Coffee Break

10:30-10:50
Optimized Sample Centering for Best Your Experimental Results. Martin Adam.

10:50-11:20
Customized multi-purpose diffractometer, inventive tool to analyze biological “calcification”. Milan Gembicky, Curtis Moore and Andrew Wang.

11:20-11:40

11:40-12:00
Lithium-ion conductivity in crystallographically aligned covalent organic frameworks. Fernando J. Uribe-Romo.
3.1.4 Apply Macromolecular Crystallography Best Practices to your Challenging Diffraction Data

Chairs: Stephen Burley, Wladek Minor

Funding provided by Anton Paar, Bristol-Myers Squibb, Bruker AXS, Dectris, HKL Research, Janssen Research & Development, Rigaku, Genentech

09:00-09:05
Welcome, Introductions, Session Objectives. Wladek Minor.

09:05-09:25
Reducing Data to |F| and \( \sigma(F) \) and Assessing Data Quality. Dominika Borek.

09:25-09:45
Space group determination. Zbyszek Otwinowski.

09:45-10:05
Getting phases from non-optimal data. Maksymilian Chruszcz.

10:05-10:30 Coffee Break

10:45-11:05
Building the Structural Model: Protein, Ligands, Metals and Other Ions. Ivan Shabalgin.

11:20-11:40
Refining the structural model: restraints, ADPs, refinement with validation. Przemyslaw Porebski.

11:55-12:15
Validating the Structure at the wwPDB. Jasmine Young.

12:15-12:25
Opportunity To Review Progress With Instructors.

12:25-12:30
Survey Monkey Request and URL Closing Remarks and Acknowledgements. Stephen Burley.

3.1.5 Advanced Surface and Interface Scattering and Applications

Chairs: Alex Hexemer, Jiang Zhang

09:00-09:30
Laser-Directed Self-Assembly of Block Copolymers Investigated with Synchrotron GISAXS. Pawel Majewski and Kevin Yager.

09:30-10:00
Investigating the attraction between hard spheres undergoing liquid-to-solid transitions. Guangcui Yuan, Junhua Luo, Yun Liu and Charles C. Han.

10:00-10:30 Coffee Break

10:30-11:00
In situ GIWAXS Analysis During Spin-Coating of Solvent and Additive Effects on Organic Electronic Thin Film Microstructure Evolution. Eric Manley, Joseph Strzalka, Tobin Marks and Lin Chen.

11:00-11:30

11:30-12:00
Scattering Analysis for GISAXS. Alexander Hexemer.
13:30-14:00
Fixed target serial crystallography at SACLA. Masaki Yamamoto.

14:00-14:30
Time-resolved structural biology over longer reactions and including complementary methods, but with less sample. Allen Orville.

14:30-15:00

15:00-15:30 Coffee Break

15:30-16:00
Exploring the dynamic of PSII at room temperature by simultaneous femtosecond X-ray spectroscopy and diffraction. Louise Lassalle, Iris Young, Mohamed Ibrahim, Ruchira Chatterjee, Sheraz Gul, Franklin Fuller, Aaron Brewster, Lacey Douthit, Ernest Pastor, Nicholas Sauter, Athina Zouni, Jan Kern, Vittal Yachandra and Junko Yano.

16:00-16:30
3.2.2 Complementary Methods

Chairs: Celestin E
Avni Bhatt, Craig Bridges
Funding provided by Art Robbins Instruments, Douglas Instruments

13:30-14:00
The influence of promiscuous metals on metalloprotein structure: Complementary techniques to separate the good, the bad, and the ugly. Edward Snell, Elizabeth Snell, Oliver Zeldin, Geoffrey Grime and Elspeth Garman.

14:00-14:30

14:30-15:00
Neutron Protein Crystallography: A Unique Tool for Probing Enzyme Mechanism. Leighton Coates.

15:00-15:30 Coffee Break

15:30-16:00

16:00-16:20
Sample absorption and background: optimizing signal/noise ratio for synchrotron and neutron diffraction. Peter Khalifah.

16:20-16:40
Probing the Heme Reactive Center of Dehaloperoxidase from Amphitrite ornata via Spectroscopic, X-ray and Neutron Crystallographic Methods. Leah Carey and Reza Ghiladi.

16:40-17:00

3.2.3 Crystal Structure and Property Prediction

Chairs: Celestin A
Mariusz Krawiec, Pete Wood
Funding provided by Boehringer Ingelheim

13:30-14:00

14:00-14:30

14:30-15:00
Solvatomorphism: the inclusion of unexpected guests. An interesting case of study of different solvates in the tecton \[\text{Pd}(1,10-\text{phen})(2,3,5,6-\text{S-C}_6\text{F}_4\text{H})_2\]. Juan Manuel German Acacio.

15:00-15:30 Coffee Break

15:30-16:00
Energy barriers and mechanisms in solid-solid phase transitions. Joost Adam van den Ende.

16:00-16:30

16:30-17:00

CANCELLED
MONDAY, MAY 29

3.2.4 Hot Structures
Chairs: Celestin D
Besty Goldsmith, Sangita Sinha

13:30-14:00
Defining Allostery and Interactions Regulating Apoptosis-Inducing Factor. John Tainer.

14:00-14:30
Structural Insight into Allosteric Inhibition of Mycobacterium tuberculosis Tryptophan Synthase. Andrzej Joachimiak.

14:30-15:00
Structural Basis For Activation of Wnk Kinases By Hydrostatic Pressure. Elizabeth Goldsmith.

15:00-15:30 Coffee Break

15:30-15:50

15:50-16:10
Mechanistic Insights into Neurotransmitter Release and Presynaptic 3 Plasticity from the Crystal Structure of Munc13-1 C1C2B-MUN. Diana R Tomchick, Junjie Xu, Marcial Camacho, Yibin Xu, Victoria Esser, Xiaoxia Liu, Thorsten Trimbuch, Yun-Zu Pan, Cong Ma, Christian Rosenmund and Josep Rizo.

16:10-16:30

16:30-16:45

16:45-17:00
The beta-barrel Assembly Machinery in Motion. Jeremy Bakelar, Anoop Narayanan and Nicholas Noinaj.

3.2.5 Crystal Growth
Chairs: Celestin B
Kenneth Harris

13:30-14:00

14:00-14:30

14:30-15:00
Origin of Regular Chiral Fluctuation or Symmetry Breaking Unique to Preferential Enrichment. Rui Tamura.

15:00-15:30 Coffee Break

15:30-15:50

15:50-16:10
Anaerobic crystallization for protein crystallography. Miki Senda, Takeru Hayashi, Masanori Hatakeyama and Toshiya Senda.

16:10-16:30
Influence of humidity on drop evaporation. Tom Friedlander, Lance Ramsey, Kasia Handing, Ellen Gualtieri, Hans van Beek.

16:30-16:45
MONDAY, MAY 29

16:45-17:00
Modeling Protein Crystal Growth Through Helical Pseudosymmetry. Travis Gallagher.

3.3.1 How do I get my Data? (Beamlines and their capabilities)
Chair: Celestin E
Asfia Huq, Tiffany Kinnibrugh
Funding provided by MacCHESS, Oak Ridge National Lab

18:30-18:38

18:38-18:46
Advanced Photon Source (APS) at the Argonne National Laboratory in Argonne, IL. Randall Winans.

18:46-18:54
Macromolecular Crystallography, Helmholtz-Zentrum Berlin (HZB-MX), Berlin, Germany. Christian Feiler.

18:54-19:02
Advanced Light Source, Lawrence Berkeley National Laboratory. Christine Beavers.

19:02-19:10
XFEL Hub at Diamond Light Source. Allen Orville.

19:10-19:18
NSLS-II, Brookhaven National Laboratory. Sanjit Ghose.

19:18-20:00  Panel Discussion.

3.3.2: Would You Publish This?
Chair: Celestin A
Danielle Gray, Carla Slebodnick
Funding provided by Crystallographic Research, Inc.

18:30-18:45
Should you publish this without publishing that? Victor Young.

18:45-19:00

19:00-19:15

19:15-19:30
Fast scans. Danielle Gray.

19:30-19:45
Space group ambiguity in Tb₃(Porphyrin)₃. Carla Slebodnick.

19:45-20:00
Disorder! Disorder! Disorder! Christine Beavers.

Business Meeting for all ACA Members
17:10pm
Celestin D
All are welcome and strongly encouraged to attend
TUESDAY, MAY 30

P4 Etter Early Career Award Presentation and Award
Chairs: Amy Sarjeant                 Celestin D

08:00-08:45am Christine Durham
Molecular mechanisms of translational control.

4.1.1 Etter Symposium
Chairs: Roberto Dos Reis, Margarita Tararina

09:00-09:15
Identification of kinetic factors that expedite solid state Fe$_2$SiS$_4$ crystal formation by in situ XRD. Zhelong Jiang, Arun Ramathan and Daniel Shoemaker.

09:15-09:30
Deciphering Composition and Connectivity in a Natural Product with Assistance of MS and 2-D NMR. Anastasiya Vinokur, Ilia A. Guzei, Derek T. Ndonteh, Paul B. White, Martha M. Vestling.

09:30-09:45
A pressure induced phase transition of 4-iodobenzonitrile. Nico Giordano and Simon Parsons.

09:45-10:00

10:00-10:30  Coffee Break

10:30-10:45
Anion Inhibition of PEPCK Manifested as Substrate Inhibition; Using Crystallographic Methods to Determine Thermodynamic Data. Matt McLeod and Todd Holyoak.

10:45-11:00

11:00-11:15
Crystallographic insight into enhanced catalytic activity of carbonic anhydrase II using “activating” ligands. Avni Bhatt, Robert McKenna, Marc Ilies.

11:15-11:30
New quaternary I4-II-IV2-VI7 chalcogenides with diamond-like structures. Stanislav Stoyko, Joshua Kotchey, Evan O’Hara and Jennifer Aitken.

11:30-11:45

11:45-12:00

4.1.2 Standard Practices in Crystallography III: Communicating Crystallographic Results
Chairs: Peter Mueller

09:00-09:30
Communicating results through crystallographic databases. Suzanna Ward, Amy Sarjeant and Matthew Lightfoot.
09:30-10:00
Should we remediate small molecule structures? If so, who should do it? Carl Schwalbe.

10:00-10:30 Coffee Break

10:30-10:50
Passive voice: You’re hiding something! Lee Daniels.

10:50-11:10

11:10-11:30
Opportunities to communicate results from challenging, non-routine macromolecular structures in open access, online journals. Diana R Tomchick.

11:30-12:00
Multiple twinning and pseudosymmetry of Z-DNA hexamer duplexes. Zhipu Luo, Zbigniew Dauter, Miroslawa Dauter.

4.1.3 Conformational Dynamics of Ligand Binding
Chairs: Barry Finzel, Michael James

09:00-09:20

09:20-09:40
Effects of engineering nonnative ligand binding into E. coli phosphoenolpyruvate carboxykinase. Henry Tang, Gregory Hura, David Shin, Steven Yannone and John Tainer.

09:40-10:00
The landscape of EPHA2 inhibition. Denis Kudlinzki, Stephanie Heinzlmeir, Bernhard Kuster and Harald Schwalbe.

10:00-10:30 Coffee Break

10:30-11:00
Structural studies of conformationally-restricted ligands binding to aspartic peptidases. Michael James, Marie Fraser, Amir Khan, Jonathan Parrish, Whitney Smith and Paul Bartlett.

11:00-11:30
Dimer asymmetry and protomer dynamics in enzyme catalysis. Emil Pai, Pedram Mehrabi, Tae Hun Kim, Zhong Ren, Adnan Sljoka, Christopher Ing, Regis Pomes and Scott Prosser.

11:30-12:00

4.1.4 In situ and Operando Measurements
Chairs: Sanjit Ghose, Wenqian Xu

09:00-09:20
In situ diffraction informed by structure prediction for the discovery of novel functional materials. John Parise.

09:20-09:40
High-speed x-ray diffraction for studying irreversible materials structure dynamics. Tao Sun and Kamel Fezzaa.
09:40-10:00

10:00-10:30 Coffee Break

10:30-10:50
In operando studies of Zr-based MOFs as nerve-agent filtration materials. Anna Plonka, Qi Wang, Wesley Gordon, Alex Balboa, Diego Troya, Weiwei Guo, Conor Sharp, Sanjaya Senanayake, John Morris, Craig Hill and Anatoly Frenkel.

10:50-11:10
Understanding the nucleation and growth of colloidal quantum dots. Michael Campos, Iva Rreza, Leslie Hamachi, Benjamin Abecassis, Emory Chan and Jonathan Owen.

11:10-11:30

11:30-11:45

11:45-12:00

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

Chairs: Celestin C Nozomi Ando, Armin Wagner
Funding provided by Dectris, MiTeGen, Rigaku, Xenocs

09:00-09:20

09:20-09:40
Adventures in Scarcity: Collecting, Processing, and Understanding Sparse Data in Serial Microcrystallography. Jennifer Wierman, Ti-Yen Lan, Michael Cook, Olivier Pare-Labrosse, Antoine Sarracini, Saeed Oghbaey, Jessica Besaw, Mark Tate, Hugh Philipp, Anling Kuo, Zachary Brown, Scott Smith, Oliver Ernst, Marian Szebenyi, Veit Elser, Dwayne Miller and Sol Gruner.

09:40-10:00

10:00-10:30 Coffee Break

10:30-11:00
Pioneering new methods for exploring macromolecular dynamics with x-rays. Lois Pollack.

11:00-11:30
Metal ions in the 70S ribosome structure: implications for the structure and structure solution. Alexey Rozov, Kamel El Omari, Iskander Khusainov, Marat Yusupov, Armin Wagner and Gulnara Yusupova.
11:30-12:00
Low background pink beam serial crystallography. Alke Meents.

4.2.1 Communicating Science to the Public

Chairs: Celestin E
Jim Fettinger, Katrina Forest

13:30-14:00

14:00-14:30
Showing that Crystallography Matters. Brian McMahon.

14:30-15:00

15:00-15:30 Coffee Break

15:30-16:00

16:00-16:30

16:30-17:00

4.2.2 General Interest II

Chairs: Celestin D
Allen Oliver, Anastasiya Vinokur

13:30-13:50
Pushing the limits of crystallography with EIGER. Marcus Mueller, Andreas Foerster.

13:50-14:10

14:10-14:30

14:30-15:00
The XtaLAB mini II: A benchtop diffractometer to enrich undergraduate education. Eric W. Reinheimer and Joseph D. Ferrara.

15:00-15:30 Coffee Break

15:30-16:00
Resolution of SPINOL by cinchona alkaloids and application of high throughput screening by solvent assist grinding. Lawrence Wan-Yin Wong, Herman Ho-Yung Sung, Jianwei Sun and Ian Duncan Williams.

15:50-16:10

16:10-16:40
Upgrade of the Advanced Crystallographic Program at ChemMatCARS. Suyin Grass Wang, Yu-Sheng Chen, Adam Stash.
TUESDAY, MAY 30

4.2.3 Structural Biology of Infectious Diseases
Chairs: Celestin A Oluwatoyin Asojo, George Lountos

13:30-14:00

14:00-14:30
Inducing Protective Antibody Response to HIV-1 with Inner Domain of gp120. Marzena Pazgier.


14:30-15:00
Deregulation mechanism of SHP2 by CagA from Helicobacter pylori. Toshiya Senda, Takeru Hayashi, Nobuhiro Suzuki, Lisa Nagase, Miki Senda and Masanori Hatakeyama.

15:00-15:30 COFFEE BREAK.

15:30-16:00

16:00-16:20
Allostery in Motion: Trypanosoma brucei enzyme brought to life by a dead paralog. Oleg Volkov, Lisa Kinch, Carson Ariagno, Xiaoyi Deng, Shihua Zhong, Nick Grishin, Diana Tomchick, Zhe Chen and Margaret Phillips.

16:20-16:40

16:40-17:00
Structural Basis of Cell-Surface Signaling by the Sigma-Regulator PupR in Pseudomonas putida. Christopher Colbert, Jaime Jensen and Sangita Sinha.

WEDNESDAY MAY 31
Planning Session for 2018 ACA Toronto
9:00am Imperial 12
4.2.4 Frontiers in SAS
Chairs: Celestin C
Jan Ilavsky, Thomas Weiss

13:30-14:00
Beyond size exclusion: Online liquid chromatography for BioSAXS. Martha Brennich, Stephanie Hutin, Katharina Weinhold, Paul Schanda and Petra Pernot.

14:00-14:30

14:30-15:00
Unique shape determination of icosahedrally symmetric particles labeled with a strong scatterer from solution x-ray scattering experiments. Youngha Hwang.

15:00-15:30 Coffee Break

15:30-16:00
Easy yet powerful biological solution SAXS instrumentation for the home lab. Soren Skou, Sergio Rodrigues, Frederic Bossan and Peter Hoghoj.

16:00-16:30
Detector upgrade drives new scientific capabilities at the Bio-SANS Instrument. Sai Venkatesh Pingali.

16:30-17:00
Insights and advantages offered by coflow to high flux solution SAXS measurements. Timothy Ryan and Nigel Kirby.

4.2.5 Advances in Structure Solution from Powder Data
Chairs: Celestin B
James Kaduk, Saul Lapidus

13:30-14:00
Structure Solution from Powder Data Using a Symmetry-Mode Parameter Set. Branton Campbell.

14:00-14:30
DiffPy-CMI - a software toolbox for structure analysis by Complex Modeling method. Pavol Juhas.

14:30-15:00

15:00-15:30 Coffee Break

15:30-16:00
Synergy between powder diffraction and density functional theory. Dilithium (citrate) crystals and their relatives. James Kaduk and Andrew Cigler.

16:00-16:30
RMCProfile: Moving closer to complex modelling. Matt Tucker.

16:30-17:00
WinPSSP: a computer program applying direct-space methods for the crystal structure solution of small molecule organic solids from X-ray powder diffraction. Silvina Pagola.
**POSTERS PRIZES**

**Pauling Poster Prizes**
The Pauling Poster Prizes were established by the ACA to honor Linus Pauling and are supported by member donations. 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 on Structural Dynamics Poster Prize**
A prize of $250 is given for excellence in research on structural determination and dynamics of systems, enabled by 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) 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.

**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. The winner will receive their personal choice of books from Springer’s extensive portfolio of titles.

**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.
POSTER HANGING INSTRUCTIONS

All posters should be displayed from 10:30 am on Saturday, May 27, until 7:30 pm on Monday, July 29. Please be present at your poster from 5:30 - 7:30 pm on the day to which you are assigned. Posters beginning with Sa present on Saturday. Posters beginning with Su present on Sunday. Poster beginning with M present on Monday.

1 - Sa

2 - Su

3 - M
New Opportunities for Structural Biology Research at SSRL and LCLS. Ana Gonzalez.

4 - Sa

6 - M
Protein crystallography analysis and ab initio structure determination with the new series of diffractometers from Rigaku Oxford Diffraction, the XtaLAB Synergy. Pierre Le Magueures.

7 - Sa
Small-molecule Crystallography in the Battery Electrolyte Development. Yulia Sevryugina, Oscar Tutusaus and Rana Mohtadi.

8 - Su
Finite-index normal subgroups of crystallographic space groups. Branton Campbell.

9 - M

10 - Sa
The real implications of reciprocal space artifacts in PDF data analysis. Daniel Olds.

11 - Su

12 - M

13 - Sa

14 - Su

15 - M
Optimizing Data Collection with the Latest Generation In-House X-Ray Sources. Matthew Benning.

16 - Sa
Insights on Uranium-Halogen Bonding Derived from Charge-Density Studies at 20 K. Christopher Gianopoulos.

17 - Su
Structural Investigation of a Novel Sulfonamide Chalcone Hybrid. Lidiane J. Michelini.

18 - M

19 - Sa
Hard X-ray-Induced Valence Tautomeric Interconversion in Cobalt-o-Dioxolene Complexes. Carlos Pinheiro.

20 - Su
Interactions of beta lactamase from MRSA and complexes of metallopolymers with penicillin like antibiotics. Swanandi Pote.

21 - M
Preparation and Characterization of Novel Solids in As-O-Mo, As(P)-O-Mo(W) and As(P)-O-Nb(W) systems. Meriem Goudjil and Nick Gerasimchuk.

22 - Sa
The Largest Crystal Structure of a Gold Nanoparticle to date - II: \(\text{Au}_{246}(\text{SC}_6\text{H}_4\text{Me})_{80}\). Kristin Kirschbaum.

23 - Su
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