



**American Crystallographic Association**

**67th Annual Meeting**

**New Orleans, LA**

**May 26 - 30, 2017**

**PROGRAM BOOK**

## Annual Meeting May 26 - 30, 2017

**Program Chairs:** Yulia Sevryugina & Ilia Guzei

**Poster Chair:** Bruce Noll

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### **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 focussed on the Cambridge Structural Database (CSD), the world's repository for all small molecule organic and metal-organic crystal structures, and its 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

## WK.04 Research Data Management

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

This workshop focusses 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

Introduction to the DDDWG 2017 Workshop on Research Data Management. John Helliwell and Brian McMahon.

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

Correct Recording of Metadata: Towards Archiving and Re-use of Raw Diffraction Images in Crystallography. Loes Kroon-Batenburg.

10:30-11:00

Research Data Management at CHESS. D. Marian Szebenyi, Devin Bougie, Aaron Finke, Richard Gillilan, Jesse Hopkins, David Schuller and Werner Sun.

11:00-11:30

Metadata for Small-Angle Scattering Measurements. Andrew Allen, Fan Zhang, Jan Il-

avsky and Pete Jemian.

13:00-13:30

Open Science and Research Data policy mandates and requirements on Principal Investigators (PIs). Simon Hodson.

13:30-14:00

Research Data Management: Structure Factors and Atomic Coordinates. Stephen Burley.

14:00-14:30

The Integrated Resource for Reproducibility in Macromolecular Crystallography (IR-RMC). Wladek Minor.

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

Dealing with the Avalanche of Data Generated in High Data Rate Macromolecular Crystallography. Jean Jakoncic, Herbert J. Bernstein, Alexei Soares, Wuxian Shi, Martin Fuchs, Robert Petkus and Robert Sweet.

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

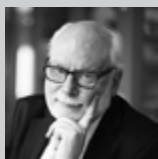
## Friday Evening Activities

### 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



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create the future." Victor Hugo**

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# SATURDAY, MAY 27

Registration Desk .....	07:30am .....	Celestin Ballroom Foyer
Speaker Ready Room .....	8:00am .....	Imperial 6 Boardroom-4th floor
Council Meeting Room.....	8:00am.....	Imperial 12
Exhibit Show .....	10:00am .....	Storyville Hall
Poster Session I.....	5:30-7:30pm .....	Storyville Hall
Undergraduate Research Symposium.....	12:00-1:00pm .....	Celestin E
Career Development.....	6:30-8:00pm .....	Celestin D

## P1.1 Poster Preview

**Chair:**

**Celestin A**

**Bill Duax**

07:45-07:51

Understanding Hysteresis in Human UDP-Glucose Dehydrogenase. Zachary Wood, Nathaniel Beattie, Phillip Gross, Renu Kadirvelraj, Nicholas Keul and Weston McDonald.

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

Neutron diffraction analysis of human manganese superoxide dismutase. Jahaun Azadmanesh, Scott Trickel, Kevin Weiss, Leighton Coates, Gloria Borgstahl.

08:09-08:15

Structural evolution and substrate specificity of Family GH31  $\alpha$ -glucosidases and their contribution to starch digestion. Marcia Chaudet, David Rose and Kyra Jones.

08:15-08:21

A Structural Study of Quinolinic Synthase, a Key Enzyme in Bacterial NAD<sup>+</sup> Biosynthesis. Neela Yennawar, Olga Esakova, Tyler Grove, Alexey Silakov, Allison Saunders, Martin McLaughlin and Squire Booker.

08:21-08:27

Monochromatic and Polychromatic Serial Crystallography at the Advanced Photon Source. Robert Fischetti.

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

Synchrotron Biosciences at National Synchrotron Light Source II: A Biomedical Technology Research Resource. Robert Sweet, Lonny Berman, Babak Andi, Herbert Bernstein, Dileep Bhogadi, Shirish Chodankar, Martin Fuchs, Yuan Gao, Vito Graziano, Nicholas Guichard, Jean Jakoncic, Edwin Lazo, Sean McSweeney, Lisa Miller, Stu Myers, Alex Soares, Dieter Schneider, Bruno Sevia Martins, Wuxian Shi, John Skinner, Vivan Stojanoff, Ryan Tappero, Yusuki Yamada and Lin Yang.

**SIG MEETINGS**

Industrial Meeting.....	12:00pm.....	Celestin C
Canadian Division Meeting .....	12:00pm.....	Celestin A
Light Source Meeting .....	5:00pm .....	Celestin C
General Interest Meeting.....	5:00pm.....	Celestin E
<b>Rigaku Reception</b> (Ticket required).....	7:00-9:00pm .....	Little Gem Saloon

07:51-07:57

Objective classification of specific radiation damage in macromolecular X-ray crystallography. Charles Bury, John McGeehan, Ian Carmichael and Elspeth Garman.

07:57-08:03

Profile fitting method to neutron time-of-flight protein single crystal diffraction data collected at iBIX. Naomine Yano.

08:03-08:09

CCP4 Web Services and Cloud Computing Developments. Ville Uski, Eugene Krissinel and Charles Ballard.

08:09-08:15

Co-Crystals of Dithieno[3,2-*a*:2',3'-*c*]phenazine Derivatives and Trimeric Perfluoro-ortho-Phenylene Mercury. Raul Castaneda, Yulia Getmanenko, Marina Fonari and Tatiana Timofeeva.

08:15-08:21

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

08:21-08:27

Mechanochemical Conversion of 11-Azaartemisinin into Pharmaceutical Cocrystals with Improved Solubility. Madiha Nisar, Richard Haynes, Herman Sung and Ian Williams.

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.

08:39-08:45

From Metric Properties to Unit Cell Databases. Lawrence C. Andrews and Herbert J. Bernstein.

**T1 Transactions I: Going Beyond PX with Cryo Electron Microscopy, Tomography & Diffraction**

**Session Chairs:** Celestin D

**Stephen Burley, Michael Rossmann**

Funding provided by Direct Electron, FEI, Gatan, JEOL USA

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.



# **SATURDAY, MAY 27**

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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

Opening Windows into the Cell: Bringing Structure to Cell Biology using Cryo-Electron Microscopy. Elizabeth Villa.

15:55-16:20

CryoEM of Molecular Machines. Wah Chiu.

16:20-16:50 Speaker Round Table

16:50-17:00

Acknowledgements and Closing Remarks. Michael G. Rossmann.

## **1.1.1 Hybrid Methods - BioSAXS**

**Session Chairs:**

**Celestin A**

**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 Bilseel and Sagar Kathuria.

10:50-11:10

Outrunning radiation damage in synchrotron biological small angle X-ray scattering. Jesse Hopkins, Clement Blanchet, Stefan Fiedler, Richard Gillilan, Cy Jeffries, Haydyn Mertens and Dmitri Svergun.

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-

ray scattering (SAXS). Soumya Govinda Remesh, Michal Hammel and Jinquan Luo.

### **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.

09:20-09:40

Advanced Total Scattering Analysis of Disordered and Nano-Crystalline Materials. Thomas Proffen.

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 understanding devices from energy conversion to superconductivity? Simon Billinge.

10:50-11:10

Chalcogenides 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, Karena 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<sub>4</sub> performance to local environment dynamics and hysteresis. Kamila Wiaderek, Olaf Borkiewicz and Karena Chapman.

11:45-12:00

DISCOVER: ORNL's Total Scattering Diffractometer for Materials Discovery. Katharine Page, Matthew Tucker and Patrick Woodward.

### **1.1.3 Utilization of Small Molecule Crystallography in Pharmaceutical Development**

**Session Chairs:**

**Celestin C**

**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

10:30-11:00

To Solvate or Not To Solvate? A Crystallographic Evaluation of the Isostructural Solvated and Non-Solvated Crystal Forms of an Active Pharmaceutical Ingredient. Michael Galella.

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 Russelburg, 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

Cuproiridsite - 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

Local structure refinements of cuboidal and spherical BaTiO<sub>3</sub> nanocrystals utilizing accurate shape effects. Tedi-Marie Usher, Daniel Olds, Jue Liu, Benard Kavey, Gabriel Caruntu and Katharine Page.

16:30-16:45

Investigation on a giant magnetoelectric effect hexaferrite via neutron scattering techniques. Yan Wu, Kun Zhai, Wei Tian, Yang Sun, Huibo Cao and Fangwei Wang.

16:45-17:00

Investigating the Local Structure and Phase Evolution of Mesoporous Gamma Alumina Using Pair Distribution Function (PDF) Analysis. Ying Zhang, Stacey Smith, Brian F. Woodfield and Daniel H. Ess.

## 1.2.3 Advances in Room Temperature Data Collection: Revealing Dynamics and Function

**Chairs:****Celestin C****Gerd Rosenbaum, Rob Thorne**

13:30-14:00

A microfluidics-based approach for serial time-resolved crystallography. Brian Mahon, Hyun Sun Cho, Friedrich Schotte and Philip Anfinrud.

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

Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin (HZB). Christian Feiler, Martin Gerlach, Ronald Forster, Christine Gless, Thomas Hauss, Michael Hellmig, Franziska Huschmann, Alexandra Kastner, Piotr Malecki, Karine Röwer, Michael Steffien, Lukas Schmuckermaier, Piotr Wilk and Manfred Weiss.

## 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

Crystal Structures of Ag(I) and Tl(I) Cyanoximates: Guide for Search for Light Insensitive Compounds, and Valuable Tool for Characterization of New Ligands. Nikolay Gerasimchuk and Jefaf Morton.

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 tetrachloridides 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

Towards establishing the structure of liquid molecular transitions metal oxides through a joint experimental and computational investigation. Paul Forster, Keith Lawler, Bradley Childs, Daniel Mast, Frederic Poineau, Alfred Sattelberger and Kenneth Czerwinski.

16:30-16:40

Rhodium(I) 2-hydroxypyridine N-oxide (hopo) complexes: synthesis, characterization and reactions. Gertruida Venter, Mohammed Elmakki, Johan Venter.

16:40-17:00

Element Mis-identification in X-ray Crystallography: A Series of Case Studies. James Donahue and Joel Mague.

Registration Desk .....	07:30am .....	Celestin Ballroom Foyer
Speaker Ready Room .....	8:00am .....	Imperial 6 Boardroom-4th floor
Council Meeting Room.....	8:00am.....	Imperial 12
Exhibit Show .....	10:00am .....	Storyville Hall
Poster Session II .....	5:30-7:30pm.....	Storyville Hall
<b>SIG MEETINGS</b>		
Young Scientist Meeting.....	12:00pm .....	Celestin D
Neutron, Materials, Powder Joint Meeting .....	12:00pm .....	Celestin B
Biological Macromolecules Meeting.....	5:00pm.....	Celestin C

**P2 Patterson Award and Lecture**  
**Amy Sarjeant, Presiding** **Celestin D**  
**08:0-08:45am**  
**The Patterson Award for a Lucky Crystallographer. Zbigniew Dauter, Argonne National Lab**

**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  
 Determination of Crystal System and Space Group. Janet Smith.

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  
 Phasing Strategies II - Molecular Replacement. Paul Adams.

11:55-12:20  
 Model Building and Structure Refinement. Paul Emsley.

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.

## SUNDAY, 28

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Andrews, Kaden Badalian, Alexei Soares, Wuxian Shi, Jean Jakoncic, Martin Fuchs, Dieter Schneider, Robert M. Sweet, Sean McSweeney, John Skinner and Yusuke Yamada.

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:**

**Paul Forster, Andrey Yakovenko**

**Celestin B**

09:00-09:30

Crystal Engineering of Hybrid Ultramicroporous Materials. Michael Zaworotko.

09:30-10:00

Structural flexibility in the solid state. Len Barbour.

10:00-10:30 Coffee Break

10:30-10:50

Development, Synthesis, and Characterization of Dithienylethenes and Their In-

corporation into Crystalline Solids. Travis Mitchell.

10:50-11:00

Nitric oxide and the Kagome lattice. Laura McCormick, Lais Aguiar, Samuel Morris, Matthew McPherson, David Cordes, Simon Teat, Alexandra Slawin, Andrelson Rinaldi and Russell Morris.

11:10-11:40

MOFs as Porous Hosts for Generating Singlet Oxygen. John MacDonald, Alwin Schwehr, Francisco Rosales Espinoza, Jiawei Lu and U Shwe Thein.

11:40-12:00

Metal-organics: A rich seam of data for knowledge mining. Peter Wood.

### 2.1.4 NMR Crystallography

**Chairs:**

**Tomislav Friscic, Manish Mehta**

Funding provided by Bruker

**Celestin C**

09:00-09:10 Introduction. Manish Mehta

09:10-09:40

Developing accurate crystallography without diffraction. James Harper.

09:40-10:00

Combined use of solid-state NMR spectroscopy and theoretical modelling as a method of structure determination. Mihails Arhangeliskis.

10:00-10:30 Coffee Break

10:30-11:00

“NMR Crystallization”: New *in-situ* NMR Techniques for Time-Resolved Monitoring of Crystallization Processes. Kenneth Harris.

11:00-11:30

NMR Crystallography in the Enzyme Active Site of Tryptophan Synthase. Leonard Mueller.

11:30-12:00

NMR Crystallography Strategies for Structure Determination of Zeolites and Layered Silicates. Darren Brouwer.

**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

$\alpha$  and  $\gamma$   $C_{60}$ -2S8 Under Pressure: A High Pressure Study of Two Polymorphs. Christine Beavers, Kamran Ghiassi, Earl O'Bannon, Alan Balch and Marilyn Olmstead.

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

Crystallographic Analysis of Analogous Silicon- and Carbon-Containing Di(Cyanate Ester)s and Tri(Cyanate Ester)s. Kamran Ghiassi, Andrew Guenther, 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

The Conservation of Allostery in *C. Elegans* UDP-Glucose Dehydrogenase. Weston McDonald, Zachary Wood, Nicholas Keul.

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-Translational 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 regulation 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

Structural analysis of MDM2-E2~ubiquitin interaction in p53 regulation. Danny Huang.

## 2.2.2 Home-Built Software

**Chairs:**

**Celestin A**

**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

Prudent Practices for Personal Programming. Larry Falvello.

14:20-14:40

Optimization and Standardization of Structure Determination Workflow in a Service Facility Using Home-Built Software. Paul Boyle.

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

ADDIE: ADvanced Diffraction Environment - A Software Environment for Analyzing Neutron Diffraction Data. Marshall McDonnell.

16:20-16:40

The Role of Home-Built Software at User Facilities: The ORNL SANS experience. Kenneth Littrell.

16:40-17:00

What is new in Olex2. Horst Puschmann and Oleg Dolomanov.

## Session 2.2.3 General Interest I

**Chairs:**

**Celestin D**

**Madushani Dharmawardana, 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

UGA-APS Soft X-ray Pilot Program at SER-CAT 22BM: Phase II - Chromatic Exploration of Uncharted Aspects of Metals in Macromolecules. Bi-Cheng Wang, John Rose, John Chrzas, Lirong Chen, Palani Kandavelu, Dayong Zhou, Unmesh Chinte, Zheng-Qing Fu, Zhongmin Jin, James Fait, Gerd Rosenbaum and Denny Mills.

14:30-14:45

Electron Crystallography of Protein Nano-Crystals. Igor Nederlof.

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

Structural and Dynamic Analysis of a Thio-redoxin-motif containing protein from the Conjugative F plasmid of Escherichia coli. Gerald Audette.

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

Sensitive detection of RNA microcrystals using SONICC imaging. Eric Zhou, Jian Xu, Ellen Gaultier, Jason Stagno, Yun-Xing Wang and Lance Ramsey.

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:**

**Kushol Gupta, Michael Hammel**

Funding provided by Anton Paar USA

**Celestin E**

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

Topological structure determination of RNA using small angle X-ray scattering. Yuba Bhandari, Linxin Fan, Xianyang Fang, George Zaki, Eric Stahlberg, Wei Ji-ang, Charles Schwieters, Jason Stagno and Yun-Xing Wang.

14:10-14:30

BECN Homologs and ATG14 Form a Conserved, Metastable Coiled-Coil to Mediate Autophagy. Sangita Sinha, Minfei Su, Yang Mei, Yue Li and Christopher Colbert.

14:30-15:00

Structure and Dynamics in Biology at the Nanoscale: X-ray Tools. Greg Hura.

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

HU multimerization shift controls nucleoid compaction. Michal Hammel, Dhar Amlanjyoti, Francis Reyes, Jian-Hua Chen, Rochelle Parpana, Henry Tang, Carolyn Larabell, John Tainer and Sankar Adhya.

## 2.2.5 Electron Diffraction of Solid State Materials

**Chairs:**

**Celestin B**

**Olaf Borkiewicz, Jim Ciston**

13:30-14:00

The Crystallography of Nanoparticles (particularly pentagonal ones). Laurence Marks.

14:00-14:30

Symmetry Group Determination and Direct Imaging of All-Inorganic Halide Perovskites  $\text{CsPbBr}_{3-x}\text{Cl}_x$ . Roberto Dos Reis, Hao Yang, Colin Ophus, Tetiana Shalapska, Gregory Bizarri, Didier Perrodin, Peter Ercius, Jim Ciston, Edith Bourret and Ulrich Dahmen.

14:30-15:00

Nanometer Resolution Mapping of Structure and Bonding in Ferroelectrics. Yu-Tsun Shao, Jian Min Zuo.

15:00-15:30 Coffee Break

15:30-16:00

Nanoscale Structure in Glasses from Coherent Electron Nanodiffraction. Paul Voyles, Jason Maldonis and Pei Zhang.

16:00-16:30

Simultaneous imaging of light and heavy elements at atomic resolution using electron ptychography and fast pixelated detectors. Hao Yang, Roberto Dos Reis, Colin Ophus,

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

16:30-17:00

Probing structural dynamics in charge-density-wave  $\text{TaSe}_{2-x}\text{Te}_x$  using ultrafast electron diffraction. Jing Tao, Junjie Li and Jun Li.

## 2.3.1 Diversity and Inclusion

**Chairs:**

**Celestin D**

**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.

### BRUKER YSIG Networking Mixer

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.



Registration Desk .....	7:30am.....	Celestin Ballroom Foyer
Speaker Ready Room .....	8:00am.....	Imperial 6 Boardroom-4th floor
Council Meeting Room.....	8:00am.....	Imperial 12
Exhibit Show .....	10:00am.....	Storyville Hall
<b>SIG MEETINGS:</b>		
Service & Small Molecule Joint SIG Meeting .....	12:00pm.....	Celestin B
Small Angle SIG Meeting .....	12:00pm.....	Celestin C
All Members Business Meeting .....	17:10pm.....	Celestin D
Poster Session III .....	5:30-7:30pm .....	Storyville Hall

**P3 Rognlie Award Presentation and Award**  
 Amy Sarjeant, Presiding Celestin D  
 08:00-08:45am  
 Community Building Challenges for the Protein Data Bank. Helen Berman, RCSB and Rutgers Univ.

**3.1.1 Materials for a Sustainable Future**  
 Chairs: Celestin A  
 Vicky Doan-Nguyen, Kamila Wiaderek

09:00-09:30  
 Multimodal Resonant Scattering for Probing Morphology, Chemistry, and Kinetics of Sustainable Materials. Cheng Wang.

09:30-10:00  
 Crystalline Products of CO<sub>2</sub> 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 chromophore precursor by crystallography and computed charge density. Alfred French, Kurt Mereiter and Thomas Rosenau.

11:40-12:00  
 Li/Ag<sub>2</sub>VO<sub>2</sub>PO<sub>4</sub> 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 Celestin D

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

09:15-09:30  
 Characterization of XANES spectra for olivine group minerals as a function of orientation and composition. Nichole R. Valdez, Mickey E. Gunter and M. Darby Dyar.

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 Cu<sub>3</sub>SbS<sub>3</sub> (skinnerite) - Cu<sub>3</sub>BiS<sub>3</sub> (wittichenite) join.. Neil Johnson, Elinor Spen-

## MONDAY, MAY 29

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cer and Nancy Ross.

11:00-11:15

Crystal structure and polymorphism of NaSrVO<sub>4</sub>: the first AIBIXVO<sub>4</sub> larnite related structure from X-ray powder diffraction data. Gwilherm Nenert, Paul O'Meara and Thomas Degen.

11:15-11:30

Applications of Laue diffraction in rock deformation measurements. Camelia Stan, Nobumichi Tamura, Martin Kunz, Kai Chen, Catherine Dejoie and Hans-Rudolf Wenk.

### 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

Grazing Incidence Diffraction with Single Crystal Diffractometer. Arturas Vailionis.

09:40-10:00

Approximating the near K-edge mass absorption coefficients of Ni using an ultrathin 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

The Use of Standard Single Crystal X-Ray Instruments to Investigate Powder Diffraction. Cary Bauer.

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:** Celestin E

**Stephen Burley, Wladek Minor**

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

09:00-09:05

Welcome, Introductions, Session Objectives. Wladek Minor.

09:05-09:25

Reducing Data to I|F| and  $\sigma(I|F|)$  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 Shabalin.

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:** Celestin C

**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

Diffraction X-ray waveguiding reveals orthogonal crystalline stratification in conjugated polymer thin films. Eliot Gann and Christopher McNeill.

11:30-12:00

Scattering Analysis for GISAXS. Alexander Hexemer.

## 3.2.1 XFEL Applications to Biological Systems

Chairs:

Celestin C

Aina Cohen, Alke Meents, George Phillips

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

Atomic structure of granulin determined from native nanocrystalline granulovirus using an X-ray free-electron laser. Cornelius Gati, Dominik Oberthuer, Oleksandr Yefanov, Richard Bunker, Peter Metcalf, Anton Barty and Henry Chapman.

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

Structures of riboswitch RNA reaction states by mix-and-inject XFEL serial crystallography. J.R. Stagno, Y. Liu, Y.R. Bhandari, C.E. Conrad, S. Panja, M. Swain, L. Fan, G. Nelson, C. Li, D.R. Wendel, T.A. White, J.D. Coe, M.O. Wiedorn, J. Knoska, D. Oberthuer, R.A. Tuckey, P. Yu, M. Dyba, S.G. Tarasov, U. Weierstall, T.D. Grant, C.D. Schwieters, J. Zhang, A.R. Ferre-D'Amare, P. Fromme, D.E.

Draper, M. Liang, M.S. Hunter, S. Boutet, K. Tan, X. Zuo, X. Ji, A. Barty, N.A. Zatsepin, H.N. Chapman, J.C.H. Spence, S.A. Woodson and Y.-X. Wang.

16:30-17:00

XFEL structures of the influenza M2 proton channel at 1.4 Å: room temperature water networks and insights into proton conduction. Jessica Thomaston, Rahel Woldeyes, Takatori Nakane, Kotaro Koivai, Ayumi Yamashita, Tomoyuki Tanaka, Toshi Arima, Jun Kobayashi, Tetsuya Masuda, Mamoru Suzuki, Michihiro Sugahara, Rie Tanaka, Eriko Nango, So Iwata, Fumiaki Yumoto, James Fraser and William Degrado.

### 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

Hybrid solution methods for tackling membrane proteins. Haydyn Mertens and Dmitri Svergun.

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

Structural information out of spectroscopy. Luke Daemen.

16:00-16:20

**CANCELLED** and: optical spectroscopy, 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

Improving the accuracy of time of flight neutron total scattering data and analysis. Daniel Olds, Richard Archibald, Thomas Proffen and Katharine Page.

### 3.2.3 Crystal Structure and Property Prediction

Chairs:

Celestin A

Mariusz Krawiec, Pete Wood

Funding provided by Boehringer Ingelheim

13:30-14:00

Structural Chemistry, Fuzzy Logic and the Law. Joel Bernstein.

14:00-14:30

Computer-guided porous materials design: from rationalization to prediction. Angeles Pulido, Anna G. Slater, Linjiang Chen, Marc A. Little, Samantha Y. Chong, Dan Holden, Tomasz Kaczorowski, Ben J. Slater, David P. McMahon, Andrew I. Cooper and Graeme M. Day.

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

Structure and electrical conductivity relationship as a function of pressure. Victoria Soghomonian, Benjamin Medina, Elinor Spencer, Christine Beavers, Nancy Ross and Carla Slebodnick.

16:30-17:00

Thermo-mechanical Responsive Crystalline Organic Semiconductor. Madushani Dharmawardana, Jeremiah Gassensmith, Raymond Welch, Gregory McCandless.



## 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

MauG catalysis: Chemistry from a distance. Carrie Wilmot, Erik Yukl and Victor Davidson.

15:50-16:10

Mechanistic Insights into Neurotransmitter Release and Presynaptic 3 Plasticity from the Crystal Structure of Munc13-1 C<sub>1</sub>C<sub>2</sub>B-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

Clustered protocadherin molecular assembly and implications for neuronal self-avoidance. Kerry M Goodman, Rotem Rubinstein, Julia Brasch, Chan Aye Thu, Fabiana Bahna, Seetha Mannepalli, Hanbin Dan, Rosemary V Sampogna, Tom Maniatis, Barry Honig and Lawrence Shapiro.

16:30-16:45

Structure/Function Analysis of *Pseudomonas putida* Nicotine Oxidoreductase. Margarita Tararina, Song Xue, Kim Janda and

Karen Allen.

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

Biologically Controlled Crystal Growth: The Image-Forming Mirror in the Eye of the Scallop. Benjamin Palmer.

14:00-14:30

Incorporation of Additives in Single Crystals - Bio-inspired approach. Yi-Yeoun Kim.

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

Flexible Ferroelectric Organic Crystals. Magdalena Owczarek.

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 Gualtier, Hans van Beek.

16:30-16:45

Automated method for iterative optimization of macromolecular crystallization screens. Daniel Wrapp, Harrison Jones, Morgan Gilman, Michael Battles, Sofia Sacerdote, Nianshuang Wang, Kasia Handing, Ellen Gualtieri, Peter Kwong and Jason McLellan.

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)**

**Chairs:** **Celestin E**

**Asfia Huq, Tiffany Kinnibrugh**

Funding provided by MacCHESS, Oak Ridge National Lab

18:30-18:38

MacChess, Cornell High Energy Synchrotron Source (CHESS). Marian Szebenyi.

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?**

**Chairs:** **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

The Fifth Phase of Cu-mip. Laura Mccormick, Samuel Morris, Simon Teat, Alexandra Slawin and Russell Morris.

19:00-19:15

Dark Secrets of "Crystal Packing and Pharmaceutical Properties of Salts of Diclofenac". Carl Schwalbe.

19:15-19:30

Fast scans. Danielle Gray.

19:30-19:45

Space group ambiguity in  $Tb_2(\text{Porphyrin})_3$ . 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

Registration Desk .....	07:30am .....	Celestin Ballroom Foyer
Speaker Ready Room .....	8:00am .....	Imperial 6 Boardroom-4th floor
Council Meeting Room .....	8:00am .....	Imperial 12
Awards Banquet .....	6:30pm .....	Storyville Hall

### 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:

Celestin D

Roberto Dos Reis, Margarita Tararina

09:00-09:15

Identification of kinetic factors that expedite solid state  $\text{Fe}_2\text{SiS}_4$  crystal formation by in situ XRD. Zhelong Jiang, Arun Ramanaathan 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, Iliia A. Guzei, Derek T. Ndinteh, 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

Negative thermal bond expansion of a molecular solid,  $\text{Tc}_2\text{O}_7$ . Daniel Mast, Bradley Childs, Keith Lawler, Frederic Poineau, Alfred Sattelberger, Kenneth Czerwinski and Paul Forster.

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

X-ray Crystallography of LpxB, a Glycosyltransferase in the Lipid A Synthesis Pathway. Thomas Bohl, John Lee, Ke Shi and Hideki Aihara.

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

Personalized biophysics of human PGM1 deficiency. Kyle Stiers.

11:45-12:00

Characterization of pH-Dependent Structural Changes in Adeno-Associated Virus by Cryo-Electron Microscopy and 3D Image Reconstruction. Justin Kurian, Antonette Bennett, Joshua Hull, Maria Janssen, Timothy Baker, Robert McKenna and Mavis Agbandje-Mckenna.

### 4.1.2 Standard Practices in Crystallography III: Communicating Crystallographic Results

Chairs:

Celestin E

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

Multivariate Analyses of Quality Metrics for Crystal Structures in the PDB Archive. Stephen K. Burley, Chenghua Shao, Huanwang Yang, John D Westbrook, Jasmine Young, Christine Zardecki.

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, Mirosława Dauter.

### 4.1.3 Conformational Dynamics of Ligand Binding

Chairs:

Celestin A

Barry Finzel, Michael James

09:00-09:20

Structure-based drug discovery for influenza by targeting the cap-snatching endonuclease activity. Gyanendra Kumar, Diane Beylkin, Wei Zhou, Jaehyeon Park, Trushar Jeevan, Chandraiah Lagiseti, Rhodri Harfoot, Richard J. Webby, Thomas R. Webb and Stephen W. White.

09:20-09:40

Effects of engineering nonnative ligand binding into *E. coli* phosphoenolpyruvate carboxykinase. Henry Tang, Gregory Hura, David Shin, Steven Yannoni 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

Targeting the Nuclear Receptor LRH-1 with Synthetic Agonists. Suzanne G. Mays, C. Denise Okafor, Richard J. Whitby, Devri-shi Goswami, Jozef Stec, Autumn R. Flynn, Michael C. Dugan, Nathan T. Jui, Patrick R. Griffin and Eric A. Ortlund.

### 4.1.4 *In situ* and Operando Measurements

Chairs:

Celestin B

Sanjit Ghose, Wenqian Xu

Funding provided by Argonne National Lab, Brookhaven National Lab, Molecular Dimensions, Oxford Cryosystems

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

Electrochemical Energy Storage Materials and Systems: Insights from *in-situ* and Operando Diffraction. Amy Marschilok, Esther Takeuchi and Kenneth Takeuchi.

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

Following *in situ* synthesis using neutron powder diffraction. Ashfia Huq, Dileka Abeysinghe, Melanie Kirkham, Robert Schmidt, Gabriel Veith and Hanno Zur Loye.

11:30-11:45

The Structure of Glycine Dihydrate: Implications for the Crystallization of Glycine from Solution and its Structure in Outer Space. Chunhua Tony Hu, Wenqian Xu and Qiang Zhu.

11:45-12:00

Crystallographic Directions of Zero Thermal Expansion in Anisotropic Oxides. Scott McCormack, William Wheeler and Waltraud Kriven.

### 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

Structure of human Fe-S assembly sub-complex. Seth Cory, Jonathan Van Vranken, Edward Brignole, Shachin Patra, Dennis Winge, Catherine Drennan, Jared Rutter and David Barondeau.

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

Structural Investigation of the HIV-1 Reverse Transcriptase Initiation Complex by HDX, SAXS, Cryo-EM, and X-ray Crystallography. Chelsy Chesterman, Steven Tuske, Jie Zheng, Youngmin Jeon, Cheng Zhang, William Cantara, Karin Musier-Forsyth, Patrick Griffin, Dmitry Lyumkis and Eddy Arnold.

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:**

**Jim Fettinger, Katrina Forest**

**Celestin E**

13:30-14:00

Demonstrating the Value of 3D Macromolecular Structures. Stephen Burley.

14:00-14:30

Showing that Crystallography Matters. Brian McMahon.

14:30-15:00

Using Social Media for #SciComm: An Interactive Tutorial. Christine Beavers.

15:00-15:30 Coffee Break

15:30-16:00

From Magic Show to Crime Scene Analysis - Getting Kids Interested in Science with Hands-on Investigations. Diane A. Dickie, Bernadette A. Hernandez-Sanchez, Richard A. Kemp, Timothy J. Boyle and Jeremiah M. Sears.

16:00-16:30

Uniqueness and You: How the Disorder of Atomic Structure Enables Your World. Katharine Page, Daniel Olds and Thomas Proffen.

16:30-17:00

Talking Science with Journalists. Catherine Meyers.

## **4.2.2 General Interest II**

**Chairs:**

**Allen Oliver, Anastasiya Vinokur**

**Celestin D**

13:30-13:50

Pushing the limits of crystallography with EIGER. Marcus Mueller, Andreas Foerster.

13:50-14:10

Teaching Outside the Classroom: Field Trips in Crystallography Education for Chemistry Students. Shao-Liang Zheng, Brian J. Malbrecht, Michael G. Campbell, Yu-Sheng Chen.

14:10-14:30

Superspace Collision: A Higher Dimensional Framework Describes Unexpected Supercell Refinement Results. Jeffrey Lovelace, Vaclav Petricek, Garib Murshudov and Gloria Borgstahl.

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

15:30-15:50

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

Crystal Structure and Physicochemical Characterization of Novel Lithium-Containing Chalcogenides. Jennifer Aitken, Ashley Weiland, Christopher Barton and Stanislav Stoyko.

16:10-16:40

Upgrade of the Advanced Crystallographic Program at ChemMatCARS. Suyin Grass Wang, Yu-Sheng Chen, Adam Stash.

## 4.2.3 Structural Biology of Infectious Diseases

**Chairs:**

**Oluwatoyin Asojo, George Lountos**

**Celestin A**

13:30-14:00

Crystal Structure of the Lassa virus surface glycoprotein. Erica Ollmann Saphire, Kathryn Hastie, Michelle Zandonatti, Luis Branco, James Robinson and Robert Garry.

14:00-14:30

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

Structure of Mycobacterium tuberculosis tryptophan synthase: a model system for allosteric inhibition. Andrzej Joachimiak, Karolina Michalska, Samantha Wellington, Partha P. Nag, Robert Jedrzejczak, Natalia I. Maltseva, Stewart L. Fisher, Stuart L. Schreiber, Deborah T. Hung.

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

Crystal structure of acid deoxyribonuclease. Jan Abendroth, Don Lorimer and Thomas Edwards.

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

Crystal structure of TAPBPR/MHC-I complex reveals insights to the mechanism of peptide editing. Jiansheng Jiang, Kannan Natarajan, Lisa Boyd, Giora Morozov, Michael

Mage and David Margulies.

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:****Jan Ilavsky, Thomas Weiss****Celestin C**

13:30-14:00

Beyond size exclusion: Online liquid chromatography for BioSAXS. Martha Brennich, Stephanie Hutin, Katharina Weinhuß, Paul Schanda and Petra Perrot.

14:00-14:30

Time-resolved SANS visualization of hierarchical structures during thermochemical reactions. Hugh O'Neill, Sai Venkatesh Pingali.

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:****James Kaduk, Saul Lapidus****Celestin B**

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

Structure solution and electronic properties of the new offset hollandite  $K_2Sn_3O_7$ . Daniel Shoemaker.

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

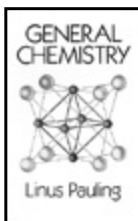
RMCPProfile: Moving closer to complex modelling. Matt Tucker.

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](http://www.rsc.org/Publishing/Journals/CE/about.asp)) shortly after the conclusion of the meeting.

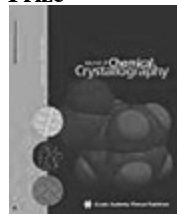


### Oxford Cryosystems Low Temperature Poster Prize

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.



### 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

The Low Temperature Crystalline Polymorphic Phase Transition of the Valpromide. Joseph Reibenspies and Nattamai Bhuvanesh.

2 - Su

Structural and functional studies of the beta-barrel assembly machinery. Jeremy Bakelar.

3 - M

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

4 - Sa

Molecular Packing Properties of Some Symmetrically Substituted Diaryl Furoxans. William Ojala, Jaya Dhami, Michael Stodolka, Samantha Whitcomb and Ryan Johnson.

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 Magueres.

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

A Structure-based Guide to Building hHint-1 Activated Nucleotide Prodrugs. Barry Finzel.

10 - Sa

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

11 - Su

Investigation of the Bacteriochlorin rings and its environment in Fenna-Matthews-Olsen antenna complex revealed by neutron and ultra-high resolution X-ray crystallography. Brinda Selvaraj.

12 - M

Absolute Configuration Determination for Light Atom Structures using Low Power Microfocus X-ray Source. Juergen Graf, Holger Ott, Tobias Stuerzer, Michael Ruf, Bruce Noll, Matthew Benning, Birger Dittrich and Carsten Michaelsen.

13 - Sa

Co-Crystals of Dithieno[3,2-a:2',3'-c]phenazine Derivatives and Trimeric Perfluoro-ortho-Phenylene Mercury. Raul Castaneda, Yulia Getmanenko, Marina Fonari and Tatiana Timofeeva.

14 - Su

Novel Boronic Acid Inhibitors of the Class D Beta-lactamase OXA-24. Rachel Springsdorf, Rachel Powers, Diane Mutete, Alina Morales, Josephine Werner, Joshua Mitchell.

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

## Posters

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- What's hiding in the PDB? Reinvestigation of structural data for the biomedically important enzymes metallo- $\beta$ -lactamases. Joanna Raczyńska, Ivan Shabalin, Alexander Wlodawer, Wladek Minor and Mariusz Jaskolski.
- 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  
Application of combined techniques for studying nano-minerals in geological system. Seungyeol Lee.
- 24 - M  
Two new cocrystals of lanthanide aquo complexes with aromatic molecules. Bulat Gabidullin, Yixin Zhang, Amalie Pialat and Muralee Murugesu.
- 25 - Sa  
Structural studies of Toll-like receptor 7. Zhikuan Zhang.
- 26 - Su  
Mechanochemical Conversion of 11-Azaarte-misinin into Pharmaceutical Cocrystals with Improved Solubility. Madiha Nisar, Richard Haynes, Herman Sung and Ian Williams.
- 27 - M  
Synchrotron Biosciences at National Synchrotron Light Source II: A Biomedical Technology Research Resource. Robert Sweet, Lonny Berman, Babak Andi, Herbert Bernstein, Dileep Bhogadi, Shirish Chodankar, Martin Fuchs, Yuan Gao, Vito Graziano, Nicholas Guichard, Jean Jakoncic, Edwin Lazo, Sean McSweeney, Lisa Miller, Stu Myers, Alex Soares, Dieter Schneider, Bruno Sevia Martins, Wuxian Shi, John Skinner, Vivian Stojanoff, Ryan Tappero, Yusuki Yamada and Lin Yang.
- 28 - Sa  
Automated data processing system for multiple small-wedge data. Keitaro Yamashita.
- 29 - Su  
Trapping conformational states of the Sida ornithine hydroxylase *in crystallo*. Ashley Campbell, John Tanner, Ritcha Mehra-Chaudhary, Julia Del Campo, Pablo Sobrado.
- 30 - M  
Crystallographic and fluorescence-based ligand binding analysis of BshC: the putative cysteine ligase in bacillithiol biosynthesis. Aaron Rosenberg, Paul Cook, Emily David, Andrew Vanduin.
- 31 - Sa  
Active-Site Protonation States in an Acyl-Enzyme Intermediate of a Class A  $\beta$ -Lactamase. Venu Gopal Vandavasi.
- 32 - Su  
The Effect of Propanone Molecule on Supramolecular Arrangement of Solvatomorphs of a Novel Anticancer Sulfonamide Chalcone. Jean M. Custodio, Wesley Fonseca Vaz, Mirian Rita Castilho de Castro, Caridad Noda Perez and Hamilton Napolitano.
- 33 - M  
Interaction Studies of Master Cardiac Transcription Factors NKX2.5 and TBX5. Saai Anugraha Tiruchendurai Suryanarayanan, Hyunjoon Nam, Shayan Ashur, Shichang Li.

34 - Sa

Phase retrieval algorithms for direct phasing of coherent nanocrystal diffraction. Joe Chen and Richard Kirian.

37 - Sa

Understanding Hysteresis in Human UDP-Glucose Dehydrogenase. Zachary Wood, Nathaniel Beattie, Phillip Gross, Renu Kadirvelraj, Nicholas Keul and Weston Mcdonald.

38 - Su

Supramolecular arrangement of two methoxy-chalcones. Hamilton Napolitano, Jean Custodio, Wesley Vaz and Eduardo Faria.

39 - M

Crystal Structure of the Chalcogen-Containing Precursors for Polymethine Dyes. Kathryn Storms, Tatiana Timofeeva, Boris Averkiev, Yulia Getmanenko.

40 - Sa

The Role of Intrinsic Disorder in Human UDP-Glucose Dehydrogenase. Nicholas Keul, Weston McDonald, Renuka Kadirvelraj, Nathan Beattie and Zachary Wood.

41 - Su

Allostery and Hysteresis are coupled in human UDP-glucose dehydrogenase. Nathaniel Beattie, Zachary Wood, Nicholas Keul, Andrew Sidlo.

42 - M

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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 have 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 Regional Associate Member of the International Union of Crystallography.

The total international membership of ACA is about 1,000 with meetings held annually. There are 12 Scientific 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 Scientist. A special division for members residing in Canada is also active. Members may join as many of these groups that are of interest 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 Ellicott St., Buffalo, NY 14203.

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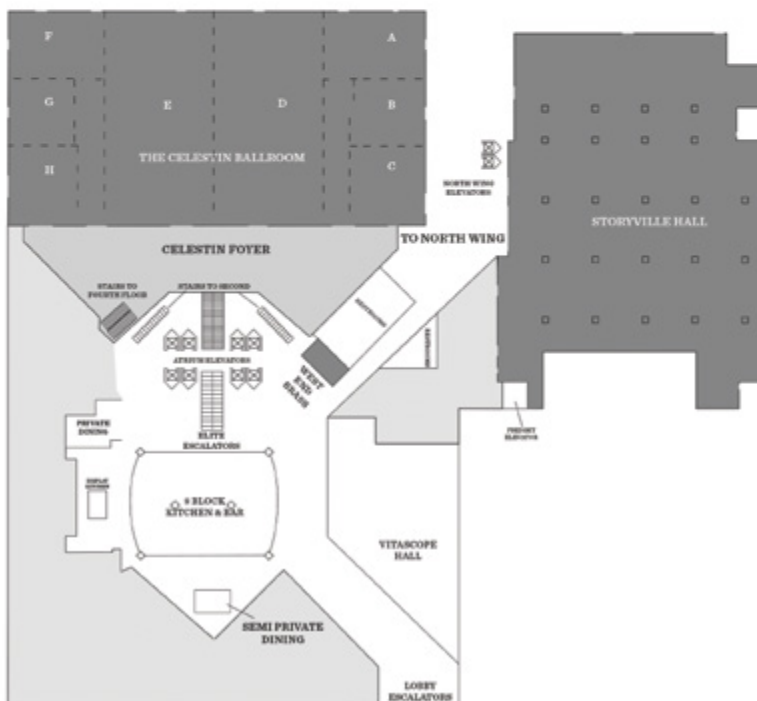
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### FLOOR PLAN

Level Three







# NOTES

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# PROGRAM AT A GLANCE

Morning		Afternoon		Evening		
WK.01 WK.02 WK.03 WK.04	CCDC - Session A - Communication CryAlis and OLEX2: From Raw Data to Publication Introduction to PHENIX Research Data Management	Strand 12 Celestin A Celestin C	CCDC - Session B - Innovation CryAlis and OLEX2 con't. Introduction to PHENIX con't. Research Data Management con't.	Strand 12 Celestin A Celestin B Celestin C	5:30 6:30 7:30	First Time Attendee and Student Meeting Orientation <i>Opening Ceremony &amp; Lecture</i> <i>Sir James Fraser Stoddart</i> Opening Reception & Exhibit Show
P1.1 P1.2 T1 1.1.1 1.1.2 1.1.3 1.1.4	Poster Preview I Poster Preview II Transactions I: Going Beyond PX... Hybrid Methods - BioSAXS Disorder, Inhomogeneity, and Local Structure Utilization of Small Molecule Cr in Pharmaceutical Development Engaging Undergraduates with Cr-Research	Celestin A Celestin C Celestin D Celestin A Celestin B Celestin C Celestin B Celestin C Celestin E	Undergraduate Research Symposium Transactions II: Going Beyond PX ... Nucleic Acids and Friends Diffuse Scattering in Complex Oxides Advances in Room Temperature Data Collection: Revealing Dynamics and Function Important Science from Small Molecules	Celestin D Celestin A Celestin B Celestin C Celestin E	SIG MEETINGS: 12:00 Industrial 12:00 Canadian Division 5:00 Light Source 5:00 General Interest 5:30 Poster Session I 6:30 Career Development 7:00 Rigata Reception	Celestin C Celestin A Celestin C Celestin E  Storyville Hall Celestin D <i>Little Gem Saloon</i>
P2 2.1.1 2.1.2 2.1.3 2.1.4 2.1.5	<i>Patterson Award - Zbigniew Dauter</i> Learn Macromolecular Cr Best Practices with Diffraction Images from a Known X-ray Structure Joint Methods for High Rate Data Processing: XFEL and Synchrotron Porous Materials NMR Crystallography Cool Structures	Celestin D Celestin E Celestin D Celestin B Celestin C Celestin A	Enzymes of Post-Translational Modifications Home-Built Software General Interest I Integrative Approaches to Structural Biology (NMR, cryoEM, SAS) Electron Diffraction of Solid State Materials	Celestin C Celestin A Celestin D Celestin E Celestin B	SIG MEETINGS: 12:00 Young Scientist 12:00 Neutron, Materials, Powder Joint 5:00 Biological/Macromolecules 5:30 Poster Session II 6:30 2.3.1 Diversity & Inclusion 8:00 Networking Mixer	Celestin D Celestin B Celestin C  Storyville Hall Celestin D Gordon Biersch Restaurant
P3 3.1.1 3.1.2 3.1.3 3.1.4 3.1.5	<i>Rognlie Award - Helen Berman</i> Materials for Sustainable Future Mineralogical Crystallography Using Standard Tools & Methods in Non-standard Ways Apply Macromolecular Cr Best Practices Advanced Surface and Interface Scattering and Applications	Celestin D Celestin A Celestin D Celestin B Celestin E Celestin C	XFEL Applications to Biological Systems Complementary Methods Crystal Structure and Property Prediction Hot Structures Crystal Growth	Celestin C Celestin E Celestin A Celestin D Celestin B	SIG MEETINGS: 12:00 Service & Small Molecule Joint 5:00 All Members Business Meeting 5:30 Poster Session III 6:30 3.3.1 How do I Get My Data? 6:30 3.3.2 Would you Publish This?	Celestin B  Celestin D Storyville Hall Celestin E Celestin A
P4 4.1.1 4.1.2 4.1.3 4.1.4 4.1.5	<i>Elder Early Career Award - Christine Durham</i> Elder Symposium Standard Practices in Cr III: Communicating Crystallographic Results Conformational Dynamics of Ligand Binding <i>In situ</i> and Operando Measurements Enabling New Science with Light Sources and Hybrid Methods	Celestin D Celestin D Celestin E Celestin A Celestin B Celestin C	Communicating Science to the Public General Interest II Structural Biology of Infectious Diseases Frontiers in SAS Advances in Structure Solution from Powder Data	Celestin E Celestin D Celestin A Celestin C Celestin B	ANNUAL AWARDS BANQUET 6:30 Cocktails 7:30 Dinner, Awards, Wood Award Lecture by James O'Brien After dinner entertainment by Dr. Jazz and	Storyville Hall
9:00	Planning Session 2018 ACA Toronto	Imperial 12				Storyville Hall Friday 7:30-10:30pm Saturday, Sunday, Monday 10:00am-7:30pm

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