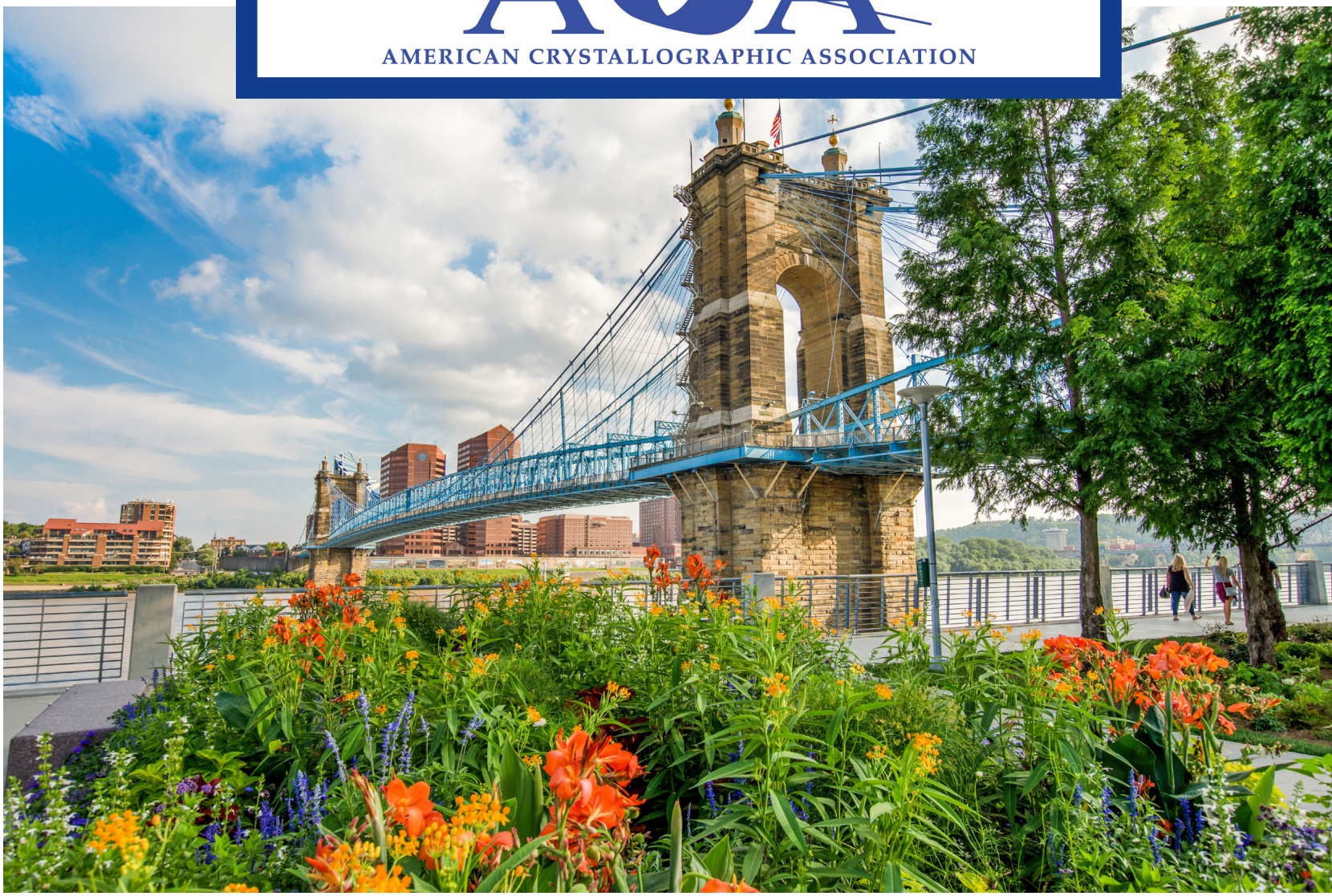
Convergent Structural Science

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION



PROGRAM BOOK

69th Annual Meeting

July 20-24, 2019

Cincinnati/Northern Kentucky

2019 MEETING SPONSORS

TRAVEL GRANT PARTNERS

The Cambridge Crystallographic Data Centre

IUCr

PDS

DIAMOND SPONSOR ($5,000+)

ThermoFisher SCIENTIFIC

RUBY SPONSORS ($2,500-$4,999)

BRUKER

DECTRIS detecting the future

MiTeGen

Rigaku oxford diffraction

EMERALD SPONSORS ($1,000-$2,499)

AIP American Institute of Physics

BioXFEL

Electron Microscopy Sciences

MOTEMPER

P

Constellation PHARMACEUTICALS

SAPPHIRE SPONSORS ($500-$999)

Victor Young Crystallographic Consultations

JEOL Solutions for Innovation

WYATT TECHNOLOGY

QUARTZ SPONSORS ($1-$499)

STOE SINCE 1887

PROTO MANUFACTURING

YSIG SPONSOR BRUKER

LANYARD SPONSOR MiTeGen

GENERAL SUPPORT SPONSOR crystals

THREE MINUTE THESIS SPONSOR ttplabtech

Welcome to the 2019 American Crystallographic Association Annual Meeting, our 69th gathering. We are glad that you are here! Thanks to the amazing efforts of the ACA Council, Program Chairs, Session Chairs, Poster Chairs and ACA Staff, as well as the hundreds of people who submitted abstracts, we have a wonderful meeting to share with you.

2019 ACA Annual Meeting Team

Program Chairs

Stephan Ginell

Vivien Yee

Poster Chairs

Louise Dawe

David Rose

Table of Contents

American Crystallographic Association, Inc.

700 Ellicott Street
Buffalo, New York 14205
www.amercrystalassn.org

COUNCIL 2019

President: **Joseph D. Ferrara**
Vice President: **Brian H. Toby**
Past President: **Lisa J. Keefe**
Canadian Rep.: **Tomislav Friscic**
Secretary: **Diana R. Tomchick**
Treasurer: **Ilia A. Guzei**
YSIG Rep.: **George Lountos**
IUCr Rep.: **Hanna Dabkowska**
Chief Executive Officer: **William L. Duax**
Chief Financial Officer: **Narasinga Rao**

STANDING COMMITTEE CHAIRS

Communications Committee:
Jim Fettinger
Education Committee:
Danielle Gray
Data, Standards & Computing Committee:
Nadia Zatsepin
Mtg. Reorganization / Enhancement Committee:
Stephan Ginell

2019 CORPORATE MEMBERS

Diamond:
- Anatrace/ Molecular Dimensions
- Art Robbins Instruments
- Bruker AXS Inc
- MiTeGen
- Rigaku Oxford Diffraction
- Stoe & Cie GmbH
- TTP Labtech Ltd

Emerald:
- American Institute of Physics
- ATPS, Inc.
- Cambridge Crystallographic Data Centre
- Charles Supper Company
- Cryo Industries Of America Inc
- Douglas Instruments Limited
- International Center for Diffraction Data
- PROTO Manufacturing Ltd.
- Rayonix LLC

Ruby:
- Anton Paar GmbH
- Dectris Ltd
- Thermo Fisher

GENERAL INFORMATION

REGISTRATION DESK

The registration desk is located outside of the Exhibit Hall on the 1st floor of the Northern Kentucky Convention Center. The registration desk will be open as follows:

Friday, July 19, 2019	6:00 PM - 8:00 PM
Saturday, July 20, 2019	7:30 AM - 7:30 PM
Sunday, July 21, 2019	7:30 AM - 5:00 PM
Monday, July 22, 2019	7:30 AM - 5:00 PM
Tuesday, July 23, 2019	7:30 AM - 5:00 PM

WIFI NETWORK

Connect to "NKYCC – Public" network and agree to the Terms and Conditions pop up for connection to the complimentary network.

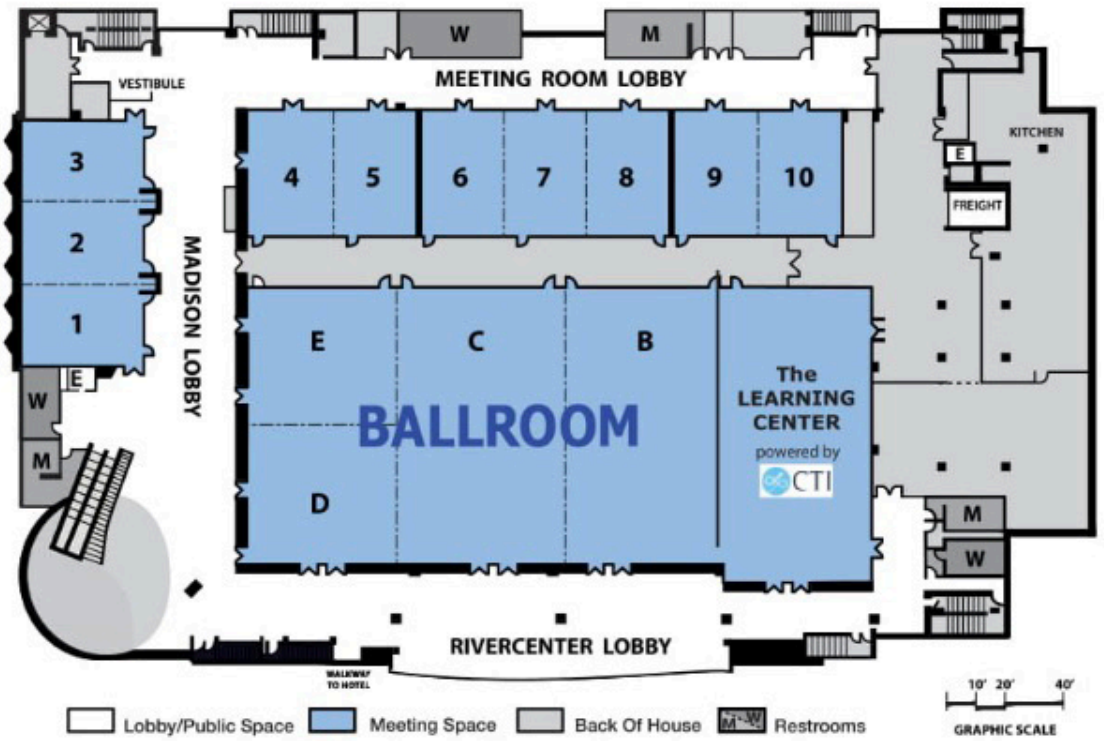
SPEAKER READY ROOM

Meeting Room #5 has been designatd as the ACA speaker ready room. This room is provided for speakers to review their talk and confirm that their presentation projects correctly. This room will be equipped with a laptop PC running windows and PowerPoint and a projector. It is mandatory that speakers review their materials the day before the presentation. If you plan on connecting a Mac, be sure to bring the proper cord.

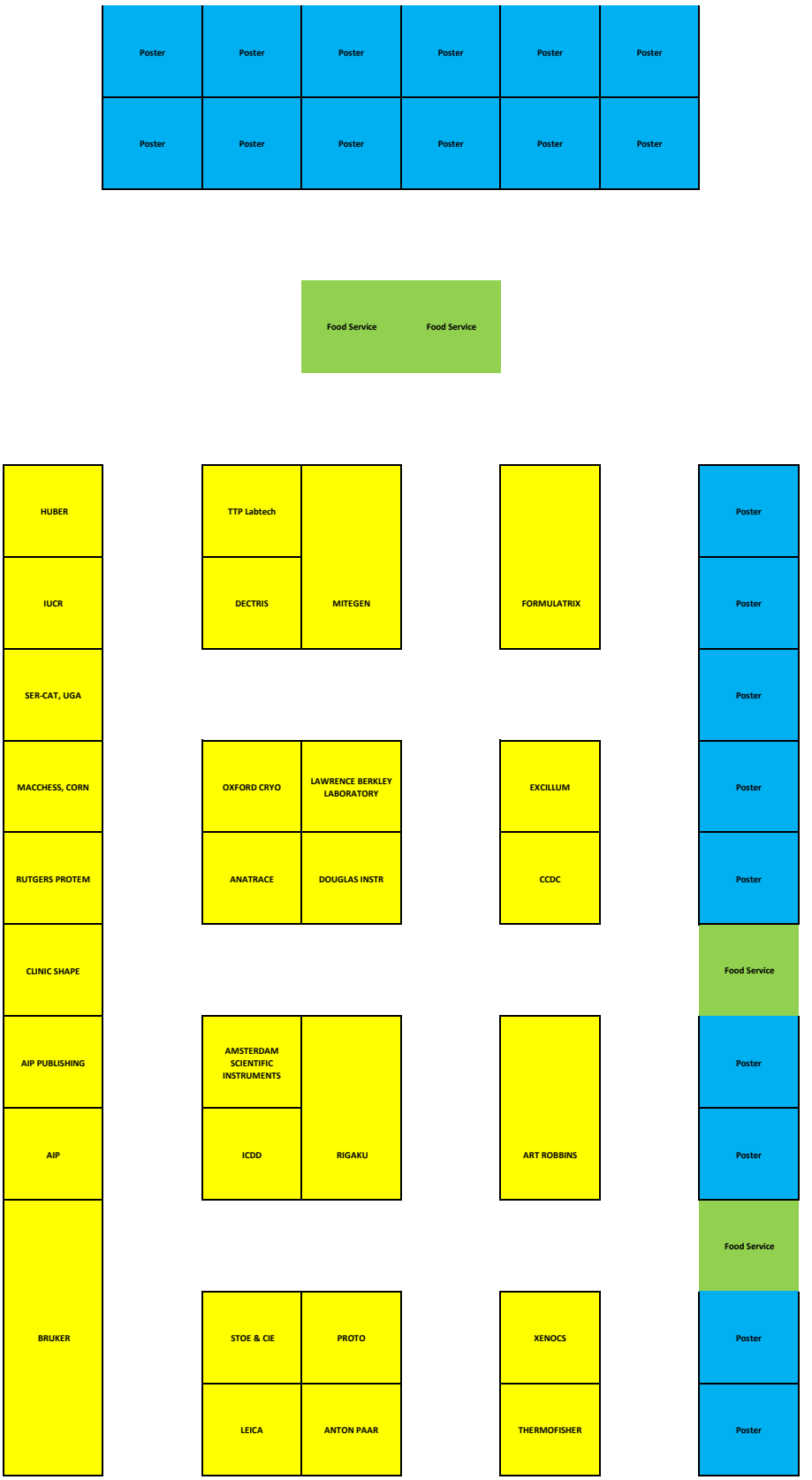
COFFEE BREAKS

Complimentary coffee breaks are available in the exhibit hall on Sunday, Monday, Tuesday, in the morning from 10:00 AM to 10:30 AM and again in the afternoon from 3:00 PM to 3:30 PM. On Wednesday the coffee break will be held in the RiverCenter Lobby from 10:00 AM to 10:30 AM and again in the afternoon from 3:00 PM to 3:30 PM.

3rd FLOOR MAP



MEETING EXHIBITORS



AIP Publishing
American Institute of Physics
Amsterdam Scientific Instruments
Anatrace/Molecular Dimensions
Anton Paar
Art Robbins Insturments
Bruker
CCDC
Clinic Shape
Dectris Ltd.
Douglas Instruments Ltd
Excillum AB
Formulatrix
Huber Diffraction USA/AXO Dresden
ICDD
IUCr
Lawrence Berkley Laboratory
Leica Microsystems
MacCHESS, Cornell University
MiTeGen
Oxford Cryosystems Inc.
Proto
Rigaku Americas
Rutgers Proteomics, RCSB Protein Data Bank
SER-CAT
STOE & Cie GmbH
Thermo Fisher Scientific
TTP Labtech
Xenocs

EXHIBIT SHOW HOURS

Saturday, July 20, 2019
7:30 PM - 10:30 PM

Sunday, July 21, 2019
10:00 AM - 12:00 PM
Closed for Lunch from 12:00 PM - 2:00 PM
2:00 PM - 7:30 PM

Monday, July 22, 2019
10:00 AM - 12:00 PM
Closed for Lunch from 12:00 PM - 2:00 PM
2:00 PM - 7:30 PM

Tuesday, July 23, 2019
10:00 AM - 12:00 PM
Closed for Lunch from 12:00 PM - 2:00 PM
2:00 PM - 7:30 PM

KEYNOTE PRESENTATION & AWARDS

Michael G. Rossmann (1930-2019):
Pioneer in Crystallography of Macromolecules & Viruses

Please join us for a Memorial Lecture to remember our member, colleague and friend.

John E. Johnson | The Scripps Research Institute, USA
Eddy Arnold | CABM, Rutgers University, USA
Hao Wu | Harvard Medical School, USA
Rui Zhao | University of Colorado, USA
S. Saif Hasan | University of Maryland School of Medicine, USA

WHEN: Saturday, July 20, 2019 @ 6:30 PM
WHERE: Ballroom B (BRB)

Trueblood Award:

Brian Toby & Robert Von Dreele

WHEN: Sunday, July 21, 2019 @8:00 AM
WHERE: Ballroom B (BRB)

Fankuchen Award:

Eaton (Ed) Lattman

WHEN: Monday, July 22, 2019 @8:00 AM
WHERE: Ballroom B (BRB)

Bau Award:

Bryan Chakoumakos

WHEN: Tuesday, July 23, 2019 @8:00 AM
WHERE: Ballroom B (BRB)

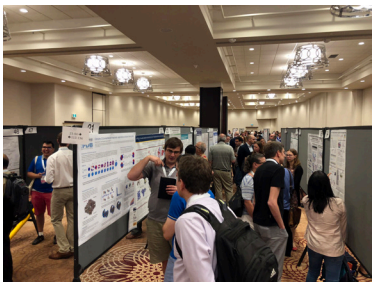
Margaret C. Etter Early Career Award:

Efrain Rodriguez

WHEN: Wednesday, July 24, 2019 @8:00 AM
WHERE: Ballroom B (BRB)

SOCIAL EVENTS & ACTIVITIES

First Time Attendee & Student Orientation
WHEN: Saturday, July 20, 2019 @ 5:30 PM – 6:30 PM
WHERE: Meeting Room 5 (MR5)



Three Minute Thesis Competition
WHEN: Sunday, July 21, 2019 @ 12:00 PM
WHERE: Ballroom B (BRB) & Ballroom C (BRC)

Poster Session #1
WHEN: Sunday, July 21, 2019 @ 5:30 PM – 7:30 PM
WHERE: Event Hall I (HALL1)

The Cambridge Crystallographic Data Centre

Dectris Lunch & Learn
WHEN: Monday, July 22, 2019 @ 12:00 PM – 1:00 PM
WHERE: Meeting Rooms 2-3 (MR23)

Three Minute Thesis FINALS!
WHEN: Monday, July 22, 2019 @ 12:00 PM
WHERE: Ballroom D (BRD)

Poster Session #2
WHEN: Monday, July 22, 2019 @ 5:30 PM – 7:30 PM
WHERE: Event Hall I (HALL1)

DECTRIS
detecting the future

CCDC Mixer
WHEN: Monday, July 22, 2019 @ 7:00 PM – 9:30 PM
WHERE: Meeting Room 3 (MR3)

YSIG Mixer (With Support From Bruker) (Ticket Required)
WHEN: Monday, July 22, 2019 @ 8:00 PM
WHERE: The Loft | Braxton Brewing (27 W 7th Covington, KY 41011)

BRUKER

All Members Business Meeting
WHEN: Tuesday, July 23, 2019 @ 5:30 PM – 6:30 PM
WHERE: Ballroom B (BRB)

Poster Session #3
WHEN: Tuesday, July 23, 2019 @ 5:30 PM – 7:30 PM
WHERE: Event Hall I (HALL1)

Banquet (Preregistration Required)
WHEN: Wednesday, July 24, 2019 @ 6:00 PM – 10:30 PM
WHERE: Belle of Cincinnati | Covington Landing Dock

SCIENTIFIC INTEREST GROUPS

Scientific Interest Groups (SIGs) are a vital part of the ACA. Each SIG represent a particular discipline within the field of crystallography, allowing members to focus on their area of specialty while retaining access to interaction with the entire range of crystallographic techniques and applications. Any member may join however many SIGs they wish. There are no additional fees association with SIG membership.

SCIENTIFIC INTEREST GROUP CHAIRS

Best Practices for Data Analysis and Archiving: **John Rose**
Biological Macromolecules: **Christopher Colbert**
Canadian Division: **David Rose**
Cryo-EM: **Rui Zhao**
Fiber Diffraction: **Joseph Orgel**
General Interest: **Joseph Tanski**
Industrial: **Angela Criswell**
Light Sources: **Ray Sierra**
Materials: **Fernando Uribe-Romo**
Neutron Scattering: **Craig Bridges**
Powder Diffraction: **Stuart Calder**
Service Crystallography: **Shao-Liang Zheng**
Small Angle Scattering: **Thomas Fitzgibbons**
Small Molecules: **Karah Knope**
Young Scientist: **Korey Carter**

Margaret C. Etter Student Lecturer Award

Each Scientific Interest Group (SIG) and the Canadian Division have the opportunity to invite one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs.

Go to www.amercrystalassn.org to find out this year's recipients and find past winners.

SCIENTIFIC INTEREST GROUP MEETINGS

Best Practices for Data Analysis & Archiving
Sunday July 21st
12:00 PM – 1:00 PM EST
Learning Center (LRNCNT)

Biological Macromolecules
Monday July 22nd
5:00 PM – 6:00 PM EST
Learning Center (LRNCNT)

Canadian Division
Sunday July 21st
5:00 PM – 6:00 PM EST
Ballroom B (BRB)

Cryo-EM
Sunday July 21st
12:00 PM – 1:00 PM EST
Ballroom D (BRD)

Fiber Diffraction
Sunday July 21st
12:00 PM – 1:00 PM EST
Meeting Room 6 (MR6)

General Interest
Monday July 22nd
12:00 PM – 1:00 PM EST
Learning Center (LRNCNT)

Industrial
Monday July 22nd
5:00 PM – 6:00 PM EST
Meeting Room 7 (MR7)

Light Sources
Monday July 22nd
12:00 PM – 1:00 PM EST
Meeting Room 7 (MR7)

[JOINT MEETING]
Materials Science, Neutron Scattering & Powder Diffraction
Monday July 22nd
5:00 PM – 6:00 PM EST
Ballroom C (BRC)

[JOINT MEETING]
Service Crystallography & Small Molecules
Monday July 22nd
12:00 PM – 1:00 PM EST
Ballroom C (BRC)

Small Angle Scattering
Sunday July 21st
12:00 PM – 1:00 PM EST
Ballroom E (BRE)

Young Scientists
Monday July 22nd
12:00 PM – 1:00 PM EST
Ballroom B (BRB)

WORKSHOPS

WK1: Advanced Structural Characterization of Nanomaterials
WHEN: Saturday, July 20, 2019 @ 8:30 AM
WHERE: Meeting Room 5 (MR5)
ORGANIZERS:
Thomas Proffen, Oak Ridge National Laboratory
Katharine Page, Oak Ridge National Laboratory

WORKSHOP #2 SPONSOR

AIP American Institute of Physics

WK2 - Accelerating Your Career Development
WHEN: Saturday, July 20, 2019 @ 1:00 PM
WHERE: Meeting Room 6 (MR6)
ORGANIZERS:
Chelsy C. Chesterman, Rutgers University
Korey Carter, Lawrence Berkeley National Laboratory
Kenneth Childers, University of Maryland

WORKSHOP #2 SPONSOR

Rigaku oxford diffraction

WK3 - Introduction to PHENIX for Electron Cryo-Microscopists
WHEN: Saturday, July 20, 2019 @ 8:30 AM
WHERE: Meeting Room 1 (MR1)
ORGANIZERS:
Paul Adams, Lawrence Berkeley Lab

WK4 - Saturday Morning Serial Crystallography: Obtaining Protein Structure from Many Crystals
WHEN: Saturday, July 20, 2019 @ 8:00 AM
WHERE: Meeting Room 2 (MR2)
ORGANIZERS:
Jennifer Wierman, SLAC National Lab, Stanford University
Aaron Finke, CHESS, Cornell University
Nicholas Sauter, Lawrence Berkeley National Lab
Graeme Winter, Diamond Light Source
Aina Cohen, SLAC National Lab, Stanford University

WORKSHOP #2 SPONSOR

Constellation PHARMACEUTICALS

WK5 - Workshop on Biological Structure Determination using Cryo-EM
WHEN:
PART 1: Monday, July 22, 2019 @ 1:30 PM
PART 2: Tuesday, July 23, 2019 @ 1:30 PM
WHERE: Ballroom E (BRE)
ORGANIZERS:
Cathy Lawson, Rutgers University
Wen Jiang, Purdue University
Michael Cianfrocco, University of Michigan

WORKSHOP #5 SPONSOR

ThermoFisher SCIENTIFIC

WK6 - Phase Identification and Materials Characterization Using Powder X-ray Diffraction
WHEN: Saturday, July 20, 2019 @ 8:30 AM
WHERE: Meeting Room 3 (MR3)
ORGANIZERS:
Thomas Blanton, ICDD
Graciela Díaz de Delgado, Universidad de Los Andes

SUNDAY, JULY 21, 2019

PL1 Trueblood Award: Brian Toby & Robert Von Dreele
Sunday, 7/21/2019 @ 8:00 AM | NKCC - Ballroom B (BRB)

TA.1: Transactions—Data Best Practices: Current State and Future Needs
Session Start Time: 09:00 AM | Room: The Learning Center
Chair(s): Nicholas Sauter, John Rose, Talapady Bhat

9:00 AM – 9:04 AM Welcome

9:04 AM – 9:28 AM
FACT and FAIR with big data allows objectivity in science: the view of crystallography. John Helliwell.

9:28 AM – 9:52 AM
Optimizing Data Quality in injector based serial millisecond crystallography. Nadia Zatsepin.

9:52 AM – 10:16 AM
FAIR data to accelerate scientific discovery at national scattering facilities. Thomas Proffen.

10:16 AM – 10:36 AM Coffee Break

10:36 AM – 11:01 AM
MicroED methodology and development. Brent Nannenga.

11:01 AM – 11:26 AM
Save the data! Diffuse scattering to shed light on structural dynamics. Michael Wall

11:26 AM – 11:51 AM
Evolving Data Standards for cryo Electron Microscopy. Catherine Lawson, Andriy Kryshtafovych, Grigore Pintilie, Helen Berman, Wah Chiu.

11:51 AM – 12:00 PM Community Discussion

1.1.1: Macromolecular Structure Under Physiological Conditions
Supporting SIGS: BioMac, Small Angle Scattering
Session Start Time: 09:00 AM: Room: Ballroom B
Chair(s): Richard Gillilan, Aina Cohen

9:00 AM – 9:05 AM Welcome - A Word About Physiology

9:05 AM - 9:30 AM
Turning Up the Heat on Dynamic Proteins: Observing molecular motion in real time with temperature-jump X-ray crystallography. Michael Thompson.

9:30 AM - 9:55 AM
Ice Formation and Solvent Nanoconfinement in Protein Crystals. Robert Thorne, David Moreau, Hakan Atakisi.

9:55 AM – 10:15 AM Coffee Break

10:15 AM - 10:40 AM
Diffraction Quality Optimization and Data Collection at Ambient Temperatures under Humidity Controlled Conditions. Silvia Russi, Jeney Wierman, Aina Cohen.

10:40 AM - 11:00 AM
Room Temperature Serial Crystallography for the Masses: How Structural Biologists Can Benefit from Crystallographers' Newest Toys. Aaron Finke.

11:00 AM - 11:20 AM
Structural consequences on transforming growth factor beta-1 activation from near therapeutic X-ray doses. Timothy Stachowski.

11:20 AM - 11:40 AM. Crystallographic and Kinetic Analysis of Temperature Variant Isozymes
Matt McLeod, Matthew McLeod, Todd Holyoak.

11:40 AM - 12:00 PM
Fixed-target serial synchrotron crystallography combined with HAG method for room temperature measurement. Takashi Kumasaka, Kazuya Hasegawa, Seiki Baba, Takashi Kawamura, Keitaro Yamashita, Kunio Hirata, Masaki Yamamoto.

1.1.2: Cutting Edge Studies using Cryo Electron Microscopes
Supporting SIGS: CryoEM, Canadian Div.
Presented With Support from Jeol & Electron Microscopy Sciences
Session Start Time: 09:00 AM | Room: Ballroom D
Chair(s): Rui Zhao, Stephen Burley

9:00 AM – 9:05 AM Introduction

9:05 AM - 9:30 AM
Recent algorithmic advances for single-particle cryo-EM. Ali Punjani.

9:30 AM - 9:55 AM
Imaging Virus Assemblies with in situ CryoEM. Peijun Zhang.

9:55 AM – 10:30 AM Coffee Break

10:30 AM - 10:55 AM
Cryo-EM of small proteins using designed assemblies as modular scaffolds. Todd Yeates, Yuxi Liu, Duc Huynh, Matthew Agdanowski.

10:55 AM - 11:20 AM
Structural Elucidation of Supramolecular Complexes in Immunity. Hao Wu.

11:20 AM - 11:35 AM
Cryo-EM structure of human ATP-citrate lyase in complex with a potent inhibitor. Jia Wei.

11:35 AM - 12:00 PM
Understanding the structure and function of spliceosome through cryoEM. Rui Zhao.

1.1.3: Morphological Characterization of Porous Materials
Supporting SIGS: Small Angle Scattering, Materials, Powder Diffraction
Session Start Time: 09:00 AM | Room: Ballroom C
Chair(s): Lilin He, Tao Li, Charl J Jafta

9:00 AM - 9:25 AM
Scattering functions of polyhedra. Byeongdu Lee.

9:25 AM - 9:42 AM
An isoreticular family of expanded photo-redox active titanium metal-organic frameworks. Demetrius Vazquez-Molina, Fernando Uribe, Zhihngyu Chen, Karena Chapman, James Harper, Matthew Logan.

9:42 AM - 9:59 AM
Structural basis of CO2 adsorption in a porous metal-organic framework material. Andrew Allen, Winnie Wong-Ng, Eric Cockayne, Jeffrey Culp, Christopher Matranga.

9:59 AM - 10:16 AM
Investigation of an in-situ chemically formed SEI from bis(fluorosulfonyl)imide based electrolyte on ordered mesoporous carbons. Charl Jafta.

10:16 AM - 10:41 AM
Model free analysis of Small Angle Scattering data of mesoporous and microporous carbons. Albrecht Petzold, Simone Mascotto, Eneli Härk, Günter Goerigk, Matthias Ballauff.

10:41 AM - 10:58 AM
Structural features of the formation of iHOF materials. Petra Bombicz, Laura Bereczki, Nora Veronika May, Roberta Palkó, Dániel Vajk Horváth, Tibor Soos, Tamás Holczbauer.

10:58 AM - 11:15 AM
Small-angle Neutron Scattering Study of Enzyme Encapsulation in Nanoporous Metal-Organic Frameworks. Lilin He, Lilin He, Xiaoliang Wang, Shuo Qian, Shengqian Ma.

11:15 AM - 11:40 AM
Advancing Cross-Scale Understanding of Reactive Fluid Induced Chemo-Morphological Changes in Multi-Phase Environments using X-Ray and Neutron Scattering Measurements. Greeshma Gadikota, Meishen Liu, Hassnain Asgar.

11:40 AM - 11:57 AM
Characterization of anisotropic nanopore structure of organic-rich marine shales in China: A SANS study. Rui Zhang, Rui Zhang, Yang Wang, Shimin Liu.

1.1.4: Crystallography in the Geosciences
Supporting SIGS: Small Molecule, Neutron, Materials, Powder Diffraction
Session Start Time: 09:00 AM | Room: Ballroom E
Chair(s): Nichole Valdez, J. Caleb Chappell

9:00 AM – 9:05 AM Introduction

9:05 AM - 9:40 AM
Predicting martian mineral compositions in situ: Crystal chemical techniques. Shaunna Morrison, Robert T Downs, David F Blake, David T Vaniman, Douglas W Ming, Allan H Treiman, Cherie N Achilles, Robert M. Hazen, Albert S Yen, Richard V Morris, Elizabeth B Rampe, Thomas F Bristow, Steve J Chipera, Nicholas Castle, Valerie Tu, Richard Walroth.

9:40 AM - 10:00 AM
Analysis of Martian Analogs Using Benchtop XRD and XRF. Gregory Schmidt.

10:00 AM – 10:30 AM Coffee Break

10:35 AM - 11:10 AM
Quartz. Rocks. Education. The crystallographic contributions of Elizabeth A. Wood. Margaret E Schott.

11:10 AM - 11:35 AM
Al-Si ordering in the incommensurately modulated structures of e-plagioclases. Shiyun Jin, Huifang Xu, Xiaoping Wang.

SUNDAY, JULY 21, 2019

11:35 AM - 12:00 PM
Successful Experimental Quantitative Charge Density Feasibility Study of Grossular Under High Pressure. Krzysztof Wozniak, Roman Gajda, Marcin Stachowicz, Anna Makal, Szymon Sutuła, Pierre Fertey, Jan Parafiniuk.

TA.2: Transactions—Data Best Practices: Current State and Future Needs
Session Start Time: 01:30 PM
Room: The Learning Center

1:15 PM - 1:30 PM
Migrating the fast_dp software package for Python 2 and 3 compatibility. Jorge A. Dias.

1:30 PM – 1:54 PM
A shared vision for macromolecular crystallography over the next five years. Andreas Förster, Clemens Schulze-Briese, Pascal Hofer.

1:54 PM – 2:18 PM
Jungfrau detector for brighter X-ray sources – MX opportunities and IT challenges. Filip Leonarski, Aldo Mozzanica, Martin Brückner, Carlos Lopez-Cuenca, Sophie Redford, Leonardo Sala, Andrej Babic, Heinrich Billich, Oliver Bunk, Bernd Schmitt, Meitian Wang.

2:18 PM – 2:42 PM
Best practices for high data-rate macromolecular crystallography (HDRMX). Herbert J.Bernstein, Lawrence C. Andrews, Jorge Diaz, Jean Jakoncic, Nicholas K. Sauter, Alexei Soares, Maciej R. Wlodek.

2:42 PM – 3:06 PM
The Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC). Wladek Minor, Marek Grabowski, Przemyslaw Porebski, Marcin Cymborowski, David Cooper.

3:06 PM – 3:30 PM Coffee Break

3:30 PM – 3:55 PM
Analysis of Electric-Field Stimulated Time-resolved X-ray Crystallography DataLigand Validation for the Protein Data Bank. Doeke Hekstra, Bo Ram Lee, Kevin M. Dalton, Rama Ranganathan.

3:55 PM – 4:20 PM
Ligand Validation for the Protein Data Bank. Stephen Burley.

4:20 PM – 4:45 PM
Challenges and opportunities in curating one million crystal structures. Amy Sarjeant, Suzanna Ward, Ian Bruno.

1.2.1: Structure Without Structure
Supporting SIGS: YSIG, BioMac, Canadian Div.
Presented With Support from Structural Dynamics & Rigaku
Session Start Time: 01:30 PM | Room: Ballroom B
Chair(s): Garrett M. Ginell, Gerald F. Audette

1:30 PM - 2:00 PM
Determining the Structure of a Protein When it Doesn't Have One. George Phillips, George Phillips.

2:00 PM - 2:20 PM
Aminoacyl-tRNA synthetases may have evolved from molten globular precursors. Zhijie Li, Charles Carter.

2:20 PM - 2:40 PM
Cooperative changes in solvent exposure identify cryptic pockets, conformational switches, and allosteric coupling. Justin Porter, Katelyn Moeder, Carrie Sibbald, Maxwell Zimmerman, Kathryn Hart, Michael Greenberg, Gregory Bowman.

2:40 PM - 3:00 PM
Future possibilities for MicroED in studying IDRs. Emma Danelius, Tamir Gonen.

3:00 PM – 3:35 PM Coffee Break

3:35 PM - 4:20 PM
The importance of measuring the solvent quality of unfolded proteins. Tobin Sosnick [Judith Flippen-Anderson Memorial Lecturer]

4:20 PM - 4:40 PM
Extreme Amyloid Polymorphism in Staphylococcus aureus Virulent PSMα Peptides. Nir Salinas.

4:40 PM - 5:00 PM
Cryo-trapping Crystal Studies of Photoreceptor PixJ Yield New Insights into its Photoconversion Mechanism. Jonathan Clinger, Mitchell Miller, Sethe Burgie, Aina Cohen, Richard Vierstra, George Phillips.

1.2.2: Crystallography at Extreme Conditions
Supporting SIGS: Small Molecule, Neutron, Materials, Powder Diffraction
Session Start Time: 01:30 PM | Room: Ballroom D
Chair(s): Camelia V. Stan, Christine M. Beavers

1:30 PM - 2:00 PM
High Pressure Studies of Zeolitic Imidozolate Frameworks (ZIFs). Nancy Ross, Jing Zhao, Athanassios Katsenis, Tomislav Friscic, Wenlin Chen.

2:00 PM - 2:30 PM
A Novel Automated Optimized, 3-D Printed Collimator Design for High Pressure Scattering Fahima Islam, Fahima Islam, Jiao Lin, Garrett Granroth.

2:30 PM - 3:00 PM
Structural Biology in the Abyss: SEC-SAXS at Deep Ocean Pressures. Richard Gillilan.

3:00 PM - 3:30 PM
Synthesis and characterization, by high pressure neutron and X-ray powder diffraction, of hybrid perovskites containing helium as a structural component. Angus Wilkinson, Brett Hester.

3:30 PM - 4:00 PM
High-pressure topotactic transition of layered CsCoO2 to stuffed cristobalite form. Branton Campbell, Branton J. Campbell, Naveed Zafar Ali, Martin Jansen.

4:00 PM - 4:30 PM
Anisotropic atomic displacement in layered materials under high pressure. Kai Zhang, Suyin Wang, Yusheng Chen.

1.2.3: Understanding Polymer Structure and Dynamics During and After Processing
Supporting SIGS: Small Angle Scattering
Session Start Time: 01:30 PM | Room: Ballroom C
Chair(s): Thomas Fitzgibbons, Ronald Jones

1:30 PM - 2:00 PM
Synchrotron X-ray Characterization and The Development of a Biomaterials Pipeline at DuPont. Juan David Londono, J David Londono, Laura Clinger.

2:00 PM - 2:20 PM
Interplay of Electrostatic Interactions, Nanoparticle Dispersion, and Ion Transport in Ionomer Nanocomposites. Allison Domhoff, Apoorv Balwani, Tyler Martin, Ronald Jones, Eric Davis.

2:20 PM - 2:40 PM
Effect of cooling rate on crystal polymorphism in beta-nucleated isotactic polypropylene as revealed by a combined WAXS/FSC analysis. Anne Gohn, Anne Gohn, Alicyn Rhoades, Nichole Wonderling, René Androsch.

2:40 PM - 3:00 PM
SAXS electron density mapping. Byeongdu Lee.

3:00 PM – 3:35 PM Coffee Break

3:35 PM - 3:55 PM
Utilizing Synchrotron Based X-ray Scattering in Polyolefin Research. Thomas Fitzgibbons, Michelle Mejia, Michael Behr, Brian Landes.

3:55 PM - 4:25 PM
Soft X-ray Characterization of Block Copolymers for Directed Self Assembly. Joseph Kline, Daniel Sunday.

1.2.4: Magnetic, quantum, and electronic correlated materials
Supporting SIGS: Neutron, Materials, Powder Diffraction
Session Start Time: 01:30 PM | Room: Ballroom E
Chair(s): Efrain E. Rodriguez, Branton Campbell

1:30 PM - 2:00 PM
Frustrated Magnetism on Nd-based Shastry-Sutherland (SS) lattices. Gabriele Sala, Matthew Stone, Andrew Christianson.

2:00 PM - 2:15 PM
Interconnected Signatures of Quantum Spin Liquid Physics Across the Barlowite Family of Quantum Magnets. Rebecca Smaha, Wei He, Jack Jiang, Charles Titus, Jiajia Wen, Young Lee.

2:15 PM - 2:30 PM
Magnetization plateaus in Tb2SrFe2O7. Huibo Cao.

2:30 PM - 3:00 PM
Magnetic PDF analysis: A tool for making geometrically frustrated magnets less frustrating. Benjamin Frandsen.

3:00 PM – 3:35 PM Coffee Break

3:30 PM - 4:00 PM
Magnetic skyrmion spin texture hosts and detection using small-angle neutron scattering. Rebecca Dally, William Ratcliff, Markus Bleuel, Lunyong Zhang, Sang-Wook Cheong, Jeffrey Lynn.

4:00 PM - 4:15 PM
Using group-subgroup relations to understand the structural instability in rutile VO2. Jared Allred, Matthew Davenport, Matthew Krogstad, Logan Whitt, Stephan Rosenkranz, Ray Osborn.

4:15 PM - 4:30 PM
Two dimensional ordering phase brought on by the destabilization of the VO2 rutile structure in V0.81Mo0.19O2. Matthew Davenport, Matthew Krogstad, Logan Whitt, Stephan Rosekranz, Ray Osborn, Jared Allred.

4:30 PM - 5:00 PM
Spin and charge stripes in trilayer nickelates. DANIEL PHELAN, Junjie Zhang, Yu-Sheng Chen, Daniel Pajerowski, Hong Zheng, Antia Botana, Leland Harriger, Jose Rodriguez-Rivera, Jacob Ruff, Nathaniel Schreiber, Bixia Wang, Mike Norman, Stephan Rosenkranz, John Mitchell.

MONDAY, JULY 22, 2019

PL2 Fankuchen Award: Eaton (Ed) Lattman
Monday, 7/22/2019 @ 8:00 AM | NKCC - Ballroom B (BRB)

2.1.1: Structure in Cancer Biology I
Supporting SIGS: BioMac, Canadian Div.
Presented With Support From: Rigaku & Wyatt Technologies
Session Start Time: 09:00 AM | Room: Ballroom B
Chair(s): Elizabeth Goldsmith, John Tainer

9:00 AM - 9:20 AM
The structure of the complex of the cytoplasmic guanine nucleotide exchange factor Ric-8A bound to Gai1. Stephen Sprang.

9:20 AM - 9:40 AM
RAF restrained and ready for RAS. Michael Eck.

9:40 AM - 10:00 AM
The STRIPAK PP2A complex couples upstream inputs to control Hippo kinase activation. Xuelian Luo, Xuelian Luo.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 10:45 AM
Inhibitors of WNK1. Elizabeth Goldsmith, Elizabeth Goldsmith, Radha Akella, Mateusz Durbacz.

10:45 AM - 11:00 AM
Apoptosis-Inducing Factor: Mechanistic Insights and Therapeutic Opportunities from a Metabolic, Allosteric Switch. Chris Brosey, Chris Brosey, Runze Shen, Kathryn Burnett, Greg Hura, John Tainer.

11:00 AM - 11:15 AM
Structure-guided discovery of dual recognition chemibodies. Xiaoshan Min.

11:15 AM - 11:30 AM
Flexible tethering of ASPP proteins facilitates PP-1c catalysis. Mark Glover.

11:30 AM - 11:45 AM
Structural and functional analyses of an allosteric Eya2 phosphatase inhibitor that has on target effects in human lung cancer cells. Rui Zhao.

11:45 AM - 12:00 PM
Structural Basis of Eukaryotic Transcription-Coupled Lesion Recognition. Dong Wang.

2.1.2: Microcrystal Electron Diffraction
Supporting SIGS: BPDAA, CryoEM
Presented with Support From ThermoFisher Scientific
Session Start Time: 09:00 AM | Room: Ballroom E
Chair(s): Tamir Gonen, Gerd Rosenbaum

9:00 AM - 9:30 AM
Structure determination by microcrystal electron diffraction. Brent Nannenga.

9:30 AM - 9:45 AM
Data collection and processing with a direct electron detector. Johan Hattne, Michael Martynowycz, Tamir Gonen.

9:45 AM - 10:00 AM
Micro Electron Diffraction is a quick and versatile tool for structure determination of macromolecules and small molecules. Alevtyna Yakushevska, Steve Reyntjens.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Development of electron diffraction techniques for ab initio crystal structure determination and phase analysis – from zeolites to proteins. Xiaodong Zou.

11:00 AM - 11:15 AM
Make MicroED an efficient tool for ultrahigh-resolution structural determination. Xueming Li, Xueming Li.

11:15 AM - 11:30 AM
Determination of structures from defined nanocrystalline regions by scanning nanobeam diffraction tomography. Marcus Gallagher-Jones, Marcus Gallagher-Jones, Karen Bustillo, Colin Ophus, Jim Ciston, Andrew Minor, Jose Rodriguez.

11:30 AM - 11:45 AM
Visualization of the core of a modified Amyloid-β polymorph with MicroED. Rebeccah Warmack.

11:45 AM - 12:00 PM
Optimizing and Evaluating Protein Microcrystallography Experiments: Strengths and weaknesses of X-rays and electrons. Michael Thompson.

2.1.3: Diffuse Scattering for Biological Structure and Dynamics
Supporting SIGS: Small Angle Scattering
Presented With Support from Mitigen, Dectris & Rigaku
Session Start Time: 09:00 AM | Room: Ballroom C
Chair(s): Steve Meisberger, Mike Wall

9:00 AM – 9:10 AM Introduction

9:10 AM - 9:35 AM
Diffuse Scattering in Small Molecule Crystallography and Beyond. Richard Welberry.

9:35 AM - 10:00 AM
Cysteine modification-gated protein dynamics explored using X-ray diffuse scattering. Mark Wilson.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 10:55 AM
Potential Implications of Time-resolved Diffuse Scattering Measurements. Eaton Lattman, Eaton Lattman.

10:55 AM - 11:05 AM
Molecular Dynamics Simulations of Protein X-ray Crystallographic Diffuse Scattering. David Wych, Michael Wall, David Mobley.

11:05 AM - 11:30 AM
Diffuse scattering in protein crystals is dominated by rigid body motions. Loes Kroon-Batenburg, Tim de Klijn, Antoine Schreurs.

11:30 AM - 11:55 AM
MD simulations of total X-ray scattering in protein crystals. David Case, Stephen Meisburger, Nozomi Ando.

11:55 AM – 12:00 PM Closing Remarks

2.1.4: Solid State NMR Crystallography
Supporting SIGS: Small Molecule, Neutron, Materials, Powder, Canadian Div.
Presented With Support from Bruker
Session Start Time: 09:00 AM | Room: Ballroom D
Chair(s): Manish Mehta, Tomislav Friscic

9:15 AM - 9:45 AM
NMR Crystallography using Quadrupolar Nuclei: Applications to Active Pharmaceutical Ingredients and Multi-Component Crystals formed by Mechanochemical Syntheses. Robert Schurko, Austin Peach, Cameron Vojvodin, Louae Abdulla, Sean Holmes, Igor Huskic, Tomislav Friscic, Robert Schurko.

9:45 AM - 10:15 AM
Hydrogen-Bonding in the Enol Tautomer of 1,3-Diketones: Insights from 2/1H Isotope Effects on NMR Parameters in the Solid State as well as Computational Chemistry. Roderick Wasylishen, Maria Matlinska, Guy Bernard, Victor Terskikh, Andreas Brinkmann.

10:15 AM - 10:45 AM
Sensitizing Solid-State NMR Spectroscopy for the Characterization of Pure and Formulated Pharmaceuticals. Aaron Rossini.

MONDAY, JULY 22, 2019

2.1.5: Crystal Structure Solution from Powder Data
Supporting SIGS: Powder, Materials, Neutrons
Session Start Time: 09:00 AM | Room: Meeting Room 7
Chair(s): Fernando Uribe-Romo, Shoji Hall

9:00 AM - 9:30 AM
Using High Pressure X-ray Powder Diffraction to Exploring Plastic and Elastic Deformations in Ultra-Hard Transition Metal Borides. Sarah Tolbert.

9:30 AM - 9:50 AM
Explore the symmetry encoding in atomic pair distribution function (PDF) with convolutional neural network (CNN). Chia-Hao Liu, Yunzhe Tao, Daniel Hsu, Qiang Du, Simon Billinge.

9:50 AM - 10:10 AM
An isoreticular family of expanded photo-redox active titanium metal-organic frameworks. Demetrius Vazquez-Molina, Fernando Uribe-romo, James Harper, Karena Chapman.

10:10 AM - 10:30 AM
Stacking Faults in Layered Electrode Materials: Developments in Structure Solutions for Diffraction Data. Alexander Brady, Hsiu-Wen Wang, Jessica Durham, Weiwei Sun, Esther Takeuchi, Kenneth Takeuchi, Amy Marschilok, Michael Naguib, Lukas Vlcek.

10:30 AM - 10:50 AM
Long range and local structure of SrxBa1-xNb2O6 (x = 0.33 and 0.67), from room temperature to 720 K. Cheng Li, Cheng Li.

2.1.6: What is a Crystal, In time & space
Supporting SIGS: Small Molecule
Session Start Time: 09:00 AM | Room: The Learning Center
Chair(s): Joseph H. Reibenspies

9:00 AM - 9:20 AM
What is a crystal: The question comes full circle. Larry R. Falvello.

9:20 AM - 9:40 AM
Continuity of Solids between Amorphous and Crystalline States – insights from Synchrotron X-ray Pair Distribution Function (SXPDF) Studies. Stephen Byrn, Gabriel de Araujo, Pam Smith, Chris Benmore.

9:40 AM - 10:00 AM
Signs of a 'Time Crystal' in a surprising place. Sean Barrett.

10:00 AM - 10:20 AM
Modulation: ordering disorder on a higher dimension. Danielle Gray.

10:20 AM - 10:40 AM
Time? Space? Crystals? Love is the answer? Love is the answer. Jason Benedict.

10:40 AM - 11:00 AM
New Insights into Organic Intergrown Polymorphic Materials. Louise N. Dawe, Zachary Schroeder, L.K. Hiscock, Camelia V. Stan, Paul D. Boyle.

11:00 AM - 11:20 AM
Crystallization and Order of Small Molecules and Nucleic Acids & their Protein Complexes. Susanna Huang, Lillian Hu.

2.2.1: Powder Difraction in Industry
Supporting SIGS: Powder, Industrial
Presented With Support from Poly Crystallography, Inc.
Session Start Time: 01:30 PM | Room: Meeting Room 7
Chair(s): James A. Kaduk, Elena Kabova

1:30 PM – 1:40 PM Introduction

1:40 PM - 2:05 PM
Current Status of X-ray Powder Diffraction in Pharmaceutical Industry. Rajni Bhardwaj.

2:05 PM - 2:30 PM
Crystal structures of commercial pharmaceuticals. James A. Kaduk, Zachary Butler, Partha Das, Amy Gindhart, Thomas Blanton.

2:30 PM - 2:55 PM
Infusible Nuclear Fuel Meta-material for Powerful Back-Flights from Far Deep Cosmic-Space Explorations. Boris Udovic.

2:55 PM – 3:30 PM Coffee Break

3:30 PM - 3:55 PM
Local magnetic cluster size identified by neutron total scattering in site-diluted spin-glass SnxFe4-xN for x=0.88. Yuanpeng Zhang, Tanja Scholz, Richard Dronskowski, Marshall McDonnell, Matthew Tucker.

3:55 PM - 4:20 PM
Powder diffraction – pragmatic, precise, or both? Elena Kabova, Elena Kabova.

2.2.2: New toys: Sources, Beamlines and Detectors
Supporting SIGS: Light Sources, Neutron, Materials, Powder, Canadian Div.
Session Start Time: 01:30 PM | Room: Ballroom C
Chair(s): Ana Gonzalez, James Holton

1:30 PM – 1:35 Introduction

1:35 PM - 2:00 PM
Wide Dynamic Range Detection and All That...Sol Gruner.

2:00 PM - 2:25 PM
Opportunities for serial femtosecond crystallography at SwissFEL. Karol Nass, Karol Nass.

2:25 PM - 2:45 PM
UHSS - A Hybrid Photon Counting Detector with a 50 Kfps Sustained Data Rate. Joseph Ferrara, Joseph Ferrara, Yasukazu Nakaye, Yasutaka Sakuma, Satoshi Mikusu, Takuto Sakumura.

2:45 PM - 3:05 PM
New Opportunities for Structural Biology Research at SSRL. Aina Cohen.

3:05 PM – 3:30 PM Coffee Break

3:30 PM - 3:55 PM
Developing a shared computing and networking infrastructure for the ALS-ENABLE structural biology program at the Advanced Light Source. Scott Classen, James Holton, Corie Ralston, Greg Hura, Jay Nix, Paul Adams.

3:55 PM - 4:15 PM
Development of next-generation high-throughput MX beamline at SPring-8. MASAKI YAMAMOTO, Kunio Hirata, Keitaro Yamashita, Seiki Baba, Kazuya Hasegawa, Naoki Sakai, Yoshiaki Kawano, Hironori Murakami, Takashi Kumasaka.

4:15 PM - 4:35 PM
CHESS-U: New beamlines, new opportunities at the Cornell High Energy Synchrotron Source. Doletha Szebenyi, Richard Gillilan, Aaron Finke.

4:35 PM - 4:55 PM
Two New Beamlines at NSLS-II for Micro-focus, Serial, and Highly Automated Macromolecular Crystallography. Wuxian Shi.

2.2.3: Locating and refining H atoms using X-rays, Neutrons, and Solid-State NMR
Supporting SIGS: Materials, Powders, Neutrons, Service Crystallography, Small Molecule
Session Start Time: 01:30 PM | Room: Ballroom D
Chair(s): James Harper, Brandon Mercado, Yu-Sheng Chen

1:30 PM - 2:00 PM
A Century after the Braggs – On Locating and Refining H-Atoms Using X-Rays and Neutrons. Krzysztof Wozniak.

2:00 PM - 2:30 PM
A solid-state NMR perspective of the hydrogen atom location and energetics in low-barrier hydrogen bonds. Gang Wu.

2:30 PM - 3:00 PM
Accurate hydrogen position from single crystal neutron diffraction. Xiaoping Wang.

MONDAY, JULY 22, 2019

3:00 PM – 3:20 PM Coffee Break

3:20 PM - 3:50 PM
Locating Hydrogen Atoms with Sensitivity Enhanced NMR Spectroscopy. Aaron Rossini.

3:50 PM - 4:20 PM
Tracking water and hydroxyl species at nanomaterial surfaces and interfaces. Katharine Page.

4:20 PM - 4:40 PM
Predicting Anisotropic Thermal Displacements from Solid-State NMR. Giovanna Pope, James Harper.

4:40 PM - 5:00 PM
Incorrect tautomer assignment in crystal structures of 1,2,4-triazoles. Carl Schwalbe.

2.2.4: General Interest l
Supporting SIGS: General Interest, YSIG
Presented With Support from Rigaku
Session Start Time: 01:30 PM | Room: Ballroom B
Chair(s): Brandon Mercado, Travis Mitchell, Matthew Brown, Joe Tanski

1:30 PM - 1:55 PM
One million structures and counting. Suzanna Ward, Amy Sarjeant.

1:55 PM - 2:20 PM
Pervasive approximate symmetry in organic P1, Z>1 structures. Carolyn P. Brock, Carolyn P. Brock.

2:20 PM - 2:40 PM
Complex form landscape of a chiral solid-solution: where does one form end and the next begin? Kevin Gagnon, Kevin J. Gagnon, Jicong Li, Ales Medek, Mettachit Navamal, Helen Shi, Sonja Sharpe.

2:40 PM - 3:00 PM
Copper cyanide polymers – new directions. Peter Corfield, Leena Rachid, Daniel Garci, Alison McCostis.

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 3:55 PM
Crystal Chemistry, Phase Diagrams, and Thermoelectric Properties of the Ca-M-Co-O (M=Sr, Zn, La, Sm, Eu, Gd, and Dy) Systems. Winnie Wong-Ng, William Laws, Saul Lapidus, Joshua Martin, James Kaduk.

3:55 PM - 4:20 PM
Selective solvent capture by molecular assemblies of diosmium sawhorses. Gregory Powell, Gregory Powell, Cynthia Powell.

4:20 PM - 4:40 PM
It's all about the numbers: Achieving best-quality data with the Bruker PHOTON III CPAD detector. Bruce Noll, Bruce C. Noll, Michael Ruf, Holger Ott, Tobias Stuerzer.

4:40 PM - 5:00 PM
Microfocus X-ray Sealed Tube Sources with Diamond Hybrid Anode Technology for Cu, Mo and Ag Radiation. Joerg Wiesmann, Juergen Graf, Paul Radcliffe.

2.2.5: Crystallization on the International Space Station
Supporting SIGS: Service Crystallography, Small Molecule, General Interest, BioMac, Materials, Powder Diffraction, Neutron
Session Start Time: 01:30 PM | Room: The Learning Center
Chair(s): Marc Giulianotti, Ken Savin

1:30 PM - 135 PM Introduction

1:35 PM - 1:55 PM
Protein Crystal Growth Research on the International Space Station: History and Future Opportunities. April Spinale.

1:55 PM - 2:15 PM
The Toledo Crystallization Box: a capillary diffusion apparatus for microgravity protein crystallization experiments. Constance Schall, Ebuka Obouji, Timothy Mueser.

2:15 PM - 2:35 PM
Use of Microgravity for the Preparation of the Large Volume Crystals Required in Neutron Diffraction Studies. Timothy Mueser, Victoria Drago, Constance Schall.

2:35 PM - 2:55 PM
ISS NL Inorganic salt crystallizations by solution evaporation and cooling. Ilia Guzei, Ilia Guzei, Stephanie Twesme, Galina Bikzhanova, April Spinale.

2:55 PM – 3:20 PM Coffee Break

3:20 PM - 3:40 PM
Taking RAS research to space. Albert Chan, Dhirendra Simanshu, Anna Maciag, Dwight Nissley.

3:40 PM - 4:00 PM
Using Microgravity at the Inernational Space Station to Lead to New Therapeutics for Taspase1: A Novel Cancer Target. Jose Manuel Martin Garcia.

4:00 PM - 4:20 PM
Effects of microgravity crystallization on a ligand-induced RNA crystal phase transition. Jason Stagno, Ping Yu, April Spinale, Paul W. Todd, Marc Giulianotti, Yun-Xing Wang.

4:20 PM - 4:40 PM
A real-time protein crystal growth approach to crystallization on the International Space Station. Kristofer Gonzalez-DeWhitt, April Spinale.

4:40 PM - 5:00 PM
Methods and devices for protein crystal growth in space. Hiroaki Tanaka, Hiroaki Tanaka, Sachiko Tanakashi, Bin Yan, Misako Koga, Yoshinobu Hashizume, Masayuki Kamo, Naoki Furubayashi, Koji Inaka.

TUESDAY, JULY 23, 2019

PL3 Bau Award: Bryan Chakoumakos
Tuesday, 7/23/2019 @ 8:00 AM | NKCC - Ballroom B (BRB)

3.1.1: Structure in Cancer Biology II
Supporting SIGS: BioMac, Canadian Div.
Presented With Support from Rigaku
Session Start Time: 09:00 AM | Room: The Learning Center
Chair(s): John Tainer, Elizabeth Goldsmith

9:00 AM - 9:20 AM
Using time-resolved crystallography and cryo-EM to investigate human DNA repair nucleases. Lorena Beese.

9:20 AM - 9:35 AM
[4Fe-4S] cluster-containing human exonuclease V acts as a novel replication fork restart factor. Chi-Lin Tsai.

9:35 AM - 9:50 AM
Structure of the XPA DNA binding domain and RPA high affinity DNA binding domains on a model NER substrate. Walter Chazin.

9:50 AM - 10:10 AM
Structural and Cellular Analyses of Cancer-Associated Mutations in DNA Repair Enzymes. Sylvie Doublié, Brian Eckenroth, Brittany Carroll, Joann Sweasy, Ash Prakash.

10:10 AM – 10:30 AM Coffee Break

10:30 AM - 10:45 AM
Protection of abasic sites during DNA replication by a stable thiazolidine protein-DNA crosslink. Brandt Eichman, Petria Thompson, Katherine Amidon, Kareem Mohni, David Cortez.

10:45 AM - 11:05 AM
A synthetic molecule stalls pre-mRNA splicing by enhancing cancer-relevant U2AF2 – RNA complexes. Clara Kielkopf, Callen Feeney, Jermaine Jenkins, Georgios Alachouzos, Zackary Falls, Ram Samudrala, Alison Frontier, Melisa Jurica.

11:05 AM - 11:20 AM
Effects of Inhibition of the Catalytic Domain of Histone Lysine Demethylase KDM5. John Horton.

11:20 AM - 11:35 AM
Structural insights into NHEJ: building up an integrated picture of the dynamic DNA double-strand breaks repair super complex. Michal Hammel, Michal Hammel.

11:35 AM - 11:50 AM
Transcription Pre-Initiation Complex with TFIIH Reveals Transcription-Ready, Repair-Regulated Helicase Machine from Combined Cryo-EM and Crystallography Datasets. John Tainer, Chunli Yan, Thomas Todd, Yuan He, Susan Tsutakawa, Ivaylo Ivanov.

3.1.2: Time - Resolved @ XFELS
Supporting SIGS: Light Sources, BioMac
Session Start Time: 09:00 AM | Room: Ballroom C
Chair(s): Marius Schmidt, Christopher Kupitz

9:00 AM - 9:20 AM
Structure of intermediates of the water oxidation reaction in photosystem II. Louise Lassalle.

9:20 AM - 9:40 AM
Photoactivation of bacterial phytochromes studied by time-resolved crystallography. Sebastian Westenhoff.

9:40 AM - 10:00 AM
Structure and dynamics of chloride ion pumping rhodopsin revealed by time resolved SFX and atomic molecular dynamics simulations. Haiguang liu.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 10:50 AM
Recent Developments in Fluctuation X-ray Scattering at X-FELs. Kanupriya Pande, Jeffrey Donatelli, Cornelius Gati, Petrus Zwart, Mark Hunter, Richard Kirian.

10:50 AM - 11:10 AM
Latest Advances on Serial Crystallography at XFELs and Synchrotron Sources. Jose Manuel Martin Garcia.

11:10 AM - 11:30 AM
Integration of Results from Time-Resolved Serial Crystallography and Spectroscopy in the Catalysis of Ceftriaxone by Beta-Lactamase. Jose L. Olmos, Jr., Hector A. Chaires, Mitchell D. Miller, George N. Phillips, Jr.

11:30 AM - 11:50 AM
Single-Particle Diffraction with the X-Ray Free Electron Laser: New Opportunities to Study Structure and Function in Biology. Peter Schwander.

3.1.3: Structural biology combining solution SAS and high resolution methods (cryoEM, MX, NMR)
Supporting SIGS: Small Angle Scattering, BioMac
Session Start Time: 09:00 AM | Room: Ballroom D
Chair(s): Jesse Hopkins, Nigel Kirby

9:00 AM - 9:30 AM
Harnessing SAXS and X-ray crystallography for high-resolution structural studies of macromolecules. Miljan Simonovic.

9:30 AM - 10:00 AM
Modeling conformationally flexible proteins with X-ray scattering and molecular simulations. Melissa Gildenberg, Todd Washington.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Insight into molecular level interactions between imidazolium based ionic liquids and cellulose combining NMR, SAXS and MD simulations. Aparna Annamraju.

11:00 AM - 11:30 AM
Mapping allosteric transitions of an enzyme with SAXS, cryo-EM, and crystallography. William Thomas, Phil Brooks, Audrey Burnim, John Bacik, JoAnne Stubbe, Jason Kaelber, James Chen, Nozomi Ando.

11:30 AM - 12:00 PM
Higher-order structures of HIV Integrase: Drug-induced Aggregates of HIV Integrase are Weak Gels. Kushol Gupta.

3.1.4: Solid State Supramolecular Chemistry and Crystal Engineering Part I
Supporting SIGS: Small Molecule, YSIG
Presented With Support from Dectris, Stoe & Proto Manufactoring
Session Start Time: 09:00 AM | Room: Ballroom B
Chair(s): Wilhelm Maximilian Hützler, Dmitriy V. Soldatov

9:00 AM – 9:10 AM Introduction

9:10 AM - 9:40 AM
From Molecular Dating to Functional Materials. Christer Aakeroy.

9:40 AM - 10:00 AM
Extending the Structural Boundaries of Quasiracemate Formation by Shape Mimicry. Kraig Wheeler, Kraig Wheeler.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Pillarplexes as molecular functional pores in the solid state. Alexander Pöthig, Alexander Pöthig.

11:00 AM - 11:20 AM
Controlling transport in triphenylene-based metal-organic frameworks. Grigorii Skorupskii, Mircea Dinca, Christopher Hendon, Benjamin Trump, Craig Brown, Thomas Kasel.

11:20 AM - 11:40 AM
Molecular switches in nanocontainers. Yael Diskin-Posner, Linda Shimon, Anton Hanopolskyi, Rafal Klajn.

11:40 AM - 12:00 PM
Experimental and Computational Solid Form Landscape of a Pharmaceutical Molecule. Rajni Bhardwaj.

TUESDAY, JULY 23, 2019

3.1.5: Functional Sustainable Materials
Supporting SIGS: Materials, Neutron, Powder Diffraction
Session Start Time: 09:00 AM | Room: Ballroom E
Chair(s): Craig A. Bridges, Matthew Logan

9:00 AM – 9:05 AM Introduction & Welcome

9:05 AM - 9:35 AM
Phase Evolution of Cathode Materials in Contact with Ceramic Electrolytes in Solid-State Batteries. Jung-Hyun Kim, Chan-Yeop Yu, Jun-Bin Choi, Venkataramani Anandan.

9:35 AM - 9:50 AM
Local environment and structure of ε-VOPO4 cycled with graphene. Kamila Wiaderek, Carrie Siu, Ieuan Seymour, Sylvia Britto, Natasha Chernova.

9:50 AM - 10:05 AM
Structure of Oxy-halide Compositions for Solid State Batteries. Margit Fabian, Istvan Tolnai.

10:05 AM – 10:35 AM Coffee Break

10:35 AM - 11:05 AM
High-symmetry metal-organic frameworks as matrices for organic-based substitutional solid solutions. Fernando Uribe-Romo, Fernando Uribe-Romo.

11:05 AM - 11:20 AM
Synthesis and X-ray Powder Diffraction Characterization of Ca12Ga14O33. Claudia Rawn, John Robert Salasin, Sabrina Schwerzler.

11:20 AM - 11:35 AM
Probing the Electrode-Electrolyte Interface with In-Operando Neutron Scattering. Craig A. Bridges, Charl Jafta, Xiaoguang Sun, Mariappan Paranthaman, William Heller, Lilin He, Grethe Jensen, Gabriel Veith, Shannon Mahurin, Sheng Dai.

11:35 AM - 11:50 AM
Mechanistic insight of ABiQ2 (A = alkali metal, Q = S, Se) using panoramic synthesis towards synthesis-by-design. Rebecca McClain, Mercouri Kanatzidis, Christos Malliakas.

11:50 AM - 12:00 PM
Structural Dynamics of Nanoalloy Catalysts inside Fuel Cells by Combined in operando X-ray Spectroscopy and Total Scattering. Valeri Petkov.

3.2.1: Application of anomalous techniques in macromolecular crystallography
Supporting SIGS: Light Sources, BioMac
Presented With Support From Dectris
Session Start Time: 01:30 PM | Room: The Learning Center
Chair(s): Toshiya Senda, Armin Wagner

1:30 PM - 2:00 PM
Optimization of macromolecular anomalous diffraction analyses. Wayne A. Hendrickson, Qun Liu.

2:00 PM - 2:20 PM
Crystallography at wavelengths longer than 2.7 Å. Kamel El Omari.

2:20 PM - 2:40 PM
MX beamline environment for measuring accurate anomalous signals from light atoms. Naohiro Matsugaki, Yusuke Yamada, Masahide Hikita, Masahiko Hiraki, Ayaka Harada, Miki Senda, Toshiya Senda.

2:40 PM - 3:00 PM
Fast native-SAD phasing at 3.75 keV with the JUNGFRAU detector. Vincent Olieric, Filip Leonarski, Naohiro Matsugaki, Sophie Redford, Aldo Mozzanica, Takashi Tomizaki, Chia-Ying Huang, Masahide Hikita, Yusuke Yamada, Toshiya Senda, Meitian Wang.

3:00 PM – 3:20 PM Coffee Break

3:20 PM - 3:40 PM
From fake news to new insights: showing what the anomalous signal and PIXE does to enhance metalloprotein biochemistry. Elspeth Garman, Geoff Grime, Edward Snell.

3:40 PM - 4:00 PM
Anomalous X-ray Diffraction studies of Ion Transport in Potassium Channels. Leighton Coates.

4:00 PM - 4:15 PM
Using the anomalous scattering of iodide to elucidate the mechanism of anionic inhibition of PEPCK. Sarah Barwell, Todd Holyoak.

4:15 PM - 4:30 PM
Crystallographic study on estimation of the valence of each of the four Mn atoms in Photosystem II using anomalous diffraction techniques. Yasufumi Umena.

4:30 PM - 4:45 PM
Single-wavelength anomalous dispersion phasing for Serial Millisecond Snapshot Crystallography. Sabine Botha.

4:45 PM - 5:00 PM
Processing simultaneously-collected MAD data from two closely-spaced (90 eV) wavelengths measured at an X-ray free electron laser. Derek Mendez, William Weis, Axel Brunger, Soichi Wakatsuki, Nicholas Sauter.

3.2.2: SAS Contrast Methods in Biology and Soft Matter
Supporting SIGS: SAS, Neutrons, Materials
Presented With Support from Rigaku
Session Start Time: 01:30 PM | Room: Ballroom C
Chair(s): Volker Urban, Kushol Gupta

1:30 PM - 2:00 PM
Deciphering the 'fuzzy' interaction of FG nucleoporins and transport factors using SANS. David Cowburn, David Cowburn, Samuel Sparks, Deniz Temel, Michael Rout.

2:00 PM - 2:30 PM
Solution structure of an intramembrane aspartyl protease by SANS. Raquel Lieberman, Swe Htet Naing, Ryan Oliver, Kevin Weiss, Volker Urban.

2:30 PM - 2:50 PM
SANS study of structures and deuterium incorporation into vegetative leaf stalks of deuterated Kale (Brassica oleracea). Zhi Yang.

2:50 PM - 3:15 PM
Medical contrast media as possible tools for SAXS contrast variation. Frank Gabel, Sylvain Engilberge, Javier Pérez, Eric Girard.

3:15 PM – 3:35 PM Coffee Break

3:35 PM - 4:05 PM
Contrast Variation with Resonant Soft X-ray Scattering for Soft Materials. Cheng Wang.

4:05 PM - 4:35 PM
Neutron-Based Static and Dynamic Biomembrane Studies Enabled by Deuterium. John Katsaras.

4:35 PM - 5:00 PM
Detecting Asymmetry and Lateral Heterogeneity Caused by Antimicrobial Peptides in Fluid Lipid Bilayer Membranes. SHUO QIAN.

3.2.3: Home-Built Software and Hardware
Supporting SIGS: Service
Presented With Support from Victor Young Crystallographic Consultations LLC
Session Start Time: 01:30 PM | Room: Ballroom D
Chair(s): Victor Young, Larry Falvello

1:30 PM - 1:50 PM
Data Analysis in Real Time with RAPDv2.0. Frank Murphy, Jon Schuermann, David Neau, Kay Perry, Kanagalaghatta Rajashankar.

1:50 PM - 2:10 PM
A Library of Shortcuts For Faster Image Making with PyMOL. Blaine Mooers.

2:10 PM - 2:30 PM
The hows and whys of Home-Built Software: Using the COSET program as a case study. Paul Boyle.

2:30 PM - 3:00 PM
Adventures with CRYSTALS: developing methods and tools with an in-house refinement code. Richard Cooper.

TUESDAY, JULY 23, 2019

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 3:50 PM
Tool time : Crystallographic tools for specimen extraction, selection and mounting. Joseph Reibenspies.

3:50 PM - 4:10 PM
Laboratory-Scale Growth of Organic Crystals from the Melt. Steven Kelley.

4:10 PM - 4:30 PM
NSF's ChemMatCARS: A Delicate Third Generation Synchrotron Radiation User facility for Chemical and Materials Crystallography. Yu-Sheng Chen, Suyin Wang, Adam Stash.

4:30 PM - 5:00 PM
ShelXle: a Qt graphical user interface for SHELXL. Christian Hübschle.

5:00 PM - 5:15 PM
MD-assisted refinement of x-ray coordinates. Oleg Mikhailovskii, Yi Xue, Nikolai Skrynnikov.

3.2.4: Solid State Supramolecular Chemistry and Crystal Engineering Part II
Supporting SIGS: Small Molecule, YSIG
Presented With Support from Stoe, Dectris & Proto Manufactoring
Session Start Time: 01:30 PM | Room: Ballroom B
Chair(s): Wilhelm Maximilian Hützler, Dmitriy V. Soldatov

1:30 PM - 2:00 PM
Crystallography informed crystal growth: A Personnel Perspective. Nicholas Blagden.

2:00 PM - 2:20 PM
Small Molecule Crystallography and Science—II. Phillip Fanwick.

2:20 PM - 2:40 PM
Structural analysis and biological profile of a novel hydroxy-chalcone. Hamilton Napolitano, Jean Custodio, Wesley Vaz, Gilberto Aquino, Bruno Neves.

2:40 PM - 3:00 PM
Designing molecular terahertz generation crystals: optimal packing could be just one carbon away. Gabriel Valdivia, Adam Wayment, Karissa Kenney, Erika Jackson, Isaac Tangen, Charles Bahr, Stacey Smith, David Michaelis, Jeremy Johnson.

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 4:00 PM
The emergent relationship between solvent-free chemistry, metal-organic frameworks and mineralogy. Tomislav Friscic, Igor Huskic.

4:00 PM - 4:20 PM
Recovery of high pressure solid forms to ambient pressure. Martin Ward, Martin Ward, Iain Oswald.

4:20 PM - 4:40 PM
Excimer emission in organic-based substitutional solid solutions of metal-organic frameworks. Wesley Newsome, Arnab Chakraborty, Amanda Morris, Fernando Uribe-Romo.

4:40 PM - 5:00 PM
Novel homo and heterometallic linear trinuclear complexes employing N-2-pyrimidylimidoyl-2-pyrimidylamidine ligands. Raúl Castañeda, Raúl Castañeda, Jaclyn Brusso.

3.3.1: Would You Publish This?
Supporting SIGS: Service, Small Molecule
Presented With Support from Rigaku & Victor Young Crystallographic Consultations LLC
Session Start Time: 05:30 PM | Room: The Learning Center
Chair(s): Danielle Gray, Carla Slebodnick

5:30 PM - 5:50 PM
Where would you publish this? Joseph Reibenspies.

5:50 PM - 6:10 PM
A pesky little thing… should I just give up? Michael Ruf, Bruce Noll, Ilia Guzei.

6:10 PM - 6:30 PM
Misbehaving twins: How messy is too messy? Stacey Smith, Gabriel Valdivia.

6:30 PM - 6:50 PM
Chirality Using Synchrotron. Richard Staples, Richard Staples.

6:50 PM - 7:10 PM
Oxidation State Assignment in Cerium Nanoclusters: Conflicting Conclusions from Single Crystal X-ray Diffraction and Spectroscopic Data. Jeff Bertke, Jennifer Wacker, Karah Knope.

7:10 PM - 7:30 PM
Reduction and Refinement Choices. Brandon Mercado, Patrick Holland, Ilija Coric.

WEDNESDAY, JULY 24, 2019

PL4 Margaret C. Etter Early Career Award: Efrain Rodriguez
Wednesday, 7/24/2019 @ 8:00 AM | NKCC - Ballroom B (BRB)

4.1.1: Central Dogma in 3D: the Legacy of Tom Steitz
Supporting SIGS: BioMac
Presented With Support from NanoTemper
Session Start Time: 09:00 AM | Room: Ballroom B
Chair(s): Phoebe A. Rice, Miljan Simonovic

9:00 AM - 9:20 AM
Structural basis for topological control of serine-family DNA recombinases. Phoebe A. Rice, Sherwin Montano, Sally Rowland, Martin Boocock, W. Marshall Stark.

9:20 AM - 9:40 AM
Peptide synthesis away from the central dogma. Martin Schmeing.

9:40 AM - 10:00 AM
Powering through ribosome assembly with molecular machines. Robin Stanley, Yu-Hua Lo, Monica Pillon.

10:00 AM - 10:20 AM
Phi29 DNA polymerase: structure and sequencing. Satwik Kamtekar.

10:20 AM - 10:40 AM
Mechanisms of Opening and Closing of the Bacterial Replicative Helicase. David Jeruzalmi.

10:40 AM - 11:00 AM
Structural studies of human selenoprotein synthesis. Miljan Simonovic.

4.1.2: Radiation damage in X-ray crystallography and cryo-EM
Supporting SIGS: Light Sources, Cryo-EM, BPDAA, BioMac
Session Start Time: 09:00 AM | Room: Ballroom D
Chair(s): Dominika Borek, Gerd Rosenbaum

9:00 AM - 9:30 AM
Using X-ray footprinting to investigate protein interactions and conformation. Corie Ralston, Sayan Gupta.

9:30 AM - 10:00 AM
Structural knowledge or X-ray damage? Dose dependent case studies on xylose isomerase revealing structural perturbations. Edward Snell, Helena Taberman, Charles Bury, Mark van der Woerd, Elspeth Garman.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Resolution and Dose Dependence of Radiation Damage in Biomolecular Systems. Hakan Atakisi, Lauren Conger, David Moreau, Robert Thorne.

11:00 AM - 11:30 AM
Painting with X-rays: virtual beams for ideal data collection. James Holton.

11:30 AM - 12:00 PM
Decomposition methods for analysis of specific radiation damage. Dominika Borek, Raquel Bromberg, Marcin Cymborowski, Przemyslaw Porebski, Wladek Minor, Zbyszek Otwinowski.

4.1.3: Cool Structures: Important Science from Small Molecule Crystallography
Supporting SIGS: Small Molecule, Service Crystallography, Canadian Div.
Session Start Time: 09:00 AM | Room: The Learning Center
Chair(s): Karah Knope, Louise Dawe

9:00 AM - 9:20 AM
Structural chemistry of actinide chloride complexes. Jennifer Wacker, Karah Knope.

9:20 AM - 9:40 AM
Investigating Complexation-Induced Chirality in Ln(III) and An(III)-3,4,3-LI(1,2-HOPO) Small Molecule and Siderocalin Protein Complexes. Korey Carter, Gauthier Deblonde, Trevor Lohrey, Peter Rupert, Marc Allaire, Dahlia An, Roland Strong, Rebecca Abergel.

9:40 AM - 10:00 AM
Hydrogen bond nets in dithionate metal salt crystals. Robert Burrow, Rafael Duarte.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Peptide solids as a home for organic species and solid state reactions. Dmitriy V. Soldatov, Aaron Smith, Farukh Ali.

11:00 AM - 11:20 AM
The dynamic behavior of polymer integrated crystals. Jake Bailey.

11:20 AM - 11:40 AM
Single Crystal Neutron Diffuse Scattering of Layered Ferromagnet Fe3-xGeTe2. Yaohua liu, Yaohua Liu, Stuart Calder, Andrew May, Yawei Hui.

11:40 AM - 12:00 PM
3D printing crystallographic data for post-printing construction. Matthew Brown, Ken Van Wieren, Hamel Tailor, David Hartling, Nabyl Merbouh.

4.1.4: In situ and Operando Characterization of Functional Films
Supporting SIGS: Neutron, Materials, Powder, Small Angle Scattering
Session Start Time: 09:00 AM | Room: Meeting Room 7
Chair(s): Joe Strzalka, Uta Ruett

9:00 AM - 9:25 AM
Real time study of local order in thin films by grazing incidence total scattering and pair distribution function analysis. Ann-Christin Dippel, Martin Roelsgaard, Bo B. Iversen, Olof Gutowski, Martin v. Zimmermann, Uta Ruett.

9:25 AM - 9:45 AM
In-Situ Gracing Incidence Wide Angle X-Ray Scattering for Hybrid Perovskite Semiconductors. Wanyi Nie.

9:45 AM - 10:00 AM
Solution-processed 2D Layered Perovksites for High Sensitivity X-ray Detector. Hsinhan Tsai, Hsinhan Tsai, Fangze Liu, Kasun Fernando, Brian Scott, Sergei Tretiak, Duc Ta Vo, Joseph Strzalka, Wanyi Nie.

10:00 AM - 10:15 AM
Probing the in-situ dynamics of structure-property evolution in hybrid perovskite thin films spincoated from complex fluids by a custom designed, beamline compatible multimodal measurement chamber. Shambhavi Pratap.

10:15 AM – 10:35 AM Coffee Break

10:35 AM - 11:00 AM
Pre-Nucleation induced Fast Ordering in Block-Copolymer Films with Dynamic Zone Annealing. Alamgir Karim, Maninderjeet Singh, Joseph Strzalka.

11:00 AM - 11:20 AM
The use of Bayesian inference in the characterization of materials and thin films. Jacob Jones.

11:20 AM - 11:40 AM
In situ GIWAXS and GISAXS studies of surfactant-templated metal oxide film formation and thermal transformation. Stephen Rankin, Arif Khan, Yuxin He, Syed Islam, Suraj Nagpure, Saikat Das, Barbara Knutson, Joseph Strzalka.

11:40 AM - 12:00 PM
Pushing Surface X-ray Probes Toward Mesoscale and Ultrafast Transient. Hua Zhou.

4.1.5: Diversity & Inclusion -- Diverse Teams Perform Better
Supporting SIGS: Industrial, YSIG
Presented With Support from Constellation Pharmaceuticals
Session Start Time: 09:00 AM | Room: Ballroom C
Chair(s): Anna Gardberg, Tooba Shamsi, Rebecca McAuliffe

9:00 AM - 9:40 AM
Inclusive STEM group dynamics using an analysis of social identities and intersectionality. Benny Chan.

WEDNESDAY, JULY 24, 2019

9:40 AM - 10:00 AM
Engaging diverse students with Crystallography Research. Oluwatoyin Asojo, Oluwatoyin Asojo.

10:00 AM – 10:30 AM Coffee Break

10:30 AM - 10:50 AM
Issues of Diversity and Inclusion for the Sciences. Laura McCullough.

10:50 AM - 11:10 AM
Creating and maintaining a diverse pipeline: a center-wide model and its application to individual laboratories. William Bauer.

11:10 AM - 11:30 AM
Extending an invitation and providing a seat at the table: Tools and methods for diversifying the work force in universities and biotechs. Tsehai Grell.

11:30 AM - 11:50 AM
Supportive Strategies in STEM Education. Bernie Santarsiero.

4.1.6: General Interest II
Supporting SIGS: General Interest, YSIG
Presented With Support from Rigaku
Session Start Time: 09:00 AM | Room: Ballroom E
Chair(s): Brandon Mercado, Travis Mitchell, Matthew Brown, Joe Tanski

9:00 AM - 9:20 AM
Co-crystallization with Dab antibody fragments: A universal method for the introduction of synthetic symmetry. Chelsy Chesterman, Eddy Arnold.

9:20 AM - 9:40 AM
Crystal Structure Of The UDP-Glucose Pyrophosphorylase From Yersinia Pestis, a Drug Target for New Anti-Plague Agents. George Lountos, George Lountos, Morgan Gibbs, Rajesh Gumpena, David Waugh.

9:40 AM - 10:00 AM
Nucleic Acid-Protein Crystallography Facilitated by Selenium-Nucleic Acids (SeNA). Zhen Huang, Andrey Kovalevsky, Qianwei Zhao, Lillian Hu.

10:00 AM - 10:20 AM
Comprehensive strategy for efficient generation of well-diffracted crystals. Miki Senda, Toshiya Senda.

10:20 AM – 10:40 AM Coffee Break

10:40 AM - 11:00 AM
Protein crystals are ~50% “solvent”. What is “solvent”? David Moreau, Hakan Atakisi, Robert Thorne.

11:00 AM - 11:20 AM
The Beta-barrel Assembly Machinery in Motion. Nicholas Noinaj.

11:20 AM - 11:40 AM
SER-CAT Scientific Highlights and Beamline Upgrade & User Program During the APS Shutdown. Bi-Cheng Wang, John Rose, John Chrzas.

11:40 AM - 12:00 PM
Protein AMPylation by an Evolutionarily Conserved Pseudokinase. Diana Tomchick, Anju Sreelatha, Samantha Yee, Victor Lopez, Brenden Park, Lisa Kinch, Sylwia Pilch, Kelly Servage, Junmei Zhang, Jenny Jiou, Monika Karasiewicz-Urbańska, Małgorzata Łobocka, Nick Grishin, Kim Orth, Roza Kucharczyk, Krzysztof Pawłowski, Vincent Tagliabracci.

4.2.1: What is the Meaning of Resolution?
Supporting SIGS: CryoEM, BioMac, BPDAA
Session Start Time: 01:30 PM | Room: Ballroom D
Chair(s): Raquel Bromberg, Zbyszek Otwinowski

1:30 PM – 1:40 PM Introduction

1:40 PM - 2:15 PM
Quantifying The Resolvability in CryoEM Structures. Wah Chiu, Greg Pinntilie.

2:15 PM - 2:50 PM
Quality vs. Resolution in Cryo-EM Maps. Scott Stagg.

2:50 PM – 3:20 PM Coffee Break

3:20 PM - 3:55 PM
Credible measures of resolution limits. Zbyszek Otwinowski, Dominika Borek, Marcin Cymborowski, Przemyslaw Porebski, Wladek Minor.

3:55 PM - 4:30 PM
Resolution, data quality metrics and diffraction limits: consolidation and outlook for macromolecular crystallography. Clemens Vonrhein, Clemens Vonrhein, Gerard Bricogne, Ian Tickle, Claus Flensburg, Rasmus Fogh, Peter Keller, Wlodek Paciorek, Andrew Sharff.

4.2.2: Structure Based Drug Design
Supporting SIGS: Industrial
Session Start Time: 01:30 PM | Room: The Learning Center
Chair(s): Thierry Fischmann Kenton Longenecker

1:30 PM - 1:52 PM
Advancing a Clinical Candidate Targeting IRAK4 from a Fragment Lead. Seungil Han.

1:52 PM - 2:14 PM
Why not wild-type IDH1? Finding novel chemical matter for the forgotten isotype. Clarissa Jakob.

2:14 PM - 2:36 PM
Lysyl-tRNA synthetase as a drug target in malaria and cryptosporidiosis. David Dranow, Donald Lorimer, Thomas Edwards, Wes Van Voorhis, Peter Myler.

2:36 PM - 2:58 PM
MicroED: Big Opportunities, Tiny Crystals. Michael Martynowycz, Michael Martynowycz.

2:58 PM – 3:28 PM Coffee Break

3:28 PM - 3:50 PM
How structural biologists and the Protein Data Bank contributed to recent US FDA new drug approvals. Stephen Burley, John Westbrook.

3:50 PM - 4:12 PM
Structure-Based Drug Design: Synergy of Structural Biology and Computational Methods. Leah Frye.

4:12 PM - 4:34 PM
Hotspots API: A toolkit for the application of Fragment Hotspot Mapping to Structure Based Drug Discovery. Peter Curran.

4:34 PM - 4:56 PM
Using Ligands with Coot. Paul Emsley, Paul Emsley.

4.2.3: Cool Structures: Important Science from Small Molecule Crystallography
Supporting SIGS: Small Molecule, Service Crystallography, Canadian Div.
Session Start Time: 01:30 PM | Room: Ballroom B
Chair(s): Jeffrey Bacon, Stacey Smith

1:30 PM - 2:00 PM
Cool Structures: Unique/Problem Structures in the Daily Life of a Staff Crystallographer. Michael Gau.

2:00 PM - 2:20 PM
FIRST-ROW TRANSITION METAL PYRIDINE / 4-PICOLINE SULFATE COMPLEXES. James Golen, Duyen Pham, Mrittika Roy, Ava Kreider-Mueller, David Manke.

2:20 PM - 2:40 PM
Structural variability and luminescence color tuning in lanthanide-organic hybrid materials. R. Lee Ayscue, Chloe Verwiel, Karah Knope.

2:40 PM - 3:00 PM
Novel Non-linear-optical Solids in As-O-Mo, As(P)-O-Mo(W) and As(P)-O-Nb(W) systems. Nick Gerasimchuk, Lauri Kivijarvi, Frank Rominger, Soma Khantra, Yu Ping, Meriem Goudjil.

WEDNESDAY, JULY 24, 2019

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 4:00 PM
Discovering New Polymorphs of Paracetamol via Melt Crystallization. Chunhua Tony Hu.

4:00 PM - 4:30 PM
Cluster-mining: An approach for determining core structures of metallic nanoparticles from atomic pair distribution function (PDF) data. Soham Banerjee, Chia-Hao Liu, Kirsten Jensen, Pavol Juhas, Jennifer Lee, Marcus Tofanelli, Christopher Ackerson, Christopher Murray, Simon Billinge.

4.2.4: In situ and Operando Measurements
Supporting SIGS: Materials, Neutron, Powder
Session Start Time: 01:30 PM | Room: Ballroom E
Chair(s): Andrey A. Yakovenko

1:30 PM - 2:00 PM
Sample Environment design for in situ and operando X-ray applications at PETRA III. Anita Ehnes.

2:00 PM - 2:20 PM
In-situ neutron PDF measurements of material in transformation: MXene and ferrite case studies. Peter Metz, Katharine Page.

2:20 PM - 2:40 PM
Adding new dimensions to in situ and operando experiments. Andreas Foerster, Andreas Förster, Clemens Schulze-Briese.

2:40 PM - 3:00 PM
Rapid Synthesis and In-situ X-ray Scattering of Vanadium Dioxide. Vicky Doan-Nguyen, Catrina Wilson, Amanda Gibson, Joshua Argo.

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 4:00 PM
In situ powder X-ray crystallography for gas sorption in metal-organic frameworks, Henry Zhi He Jiang, Julia Oktawiec, Rodolfo Torres-Gavosto, Eugene Kim, Benjamin A. Trump, Craig M. Brown, Jeffrey R. Long.

4:00 PM - 4:20 PM
In situ ambient-pressure synthesis of nonstoichiometric Ag3O: Phase abundance, unit-cell parameters, and c/a as a function of temperature. Paul Schields, Nicholas Dunwoody, David Field.

4:20 PM - 4:40 PM
Thermal Characterization of As Synthesized Nano Ceria. Jonathan Hanson, Milinda Abeykoon, Yuga Columbia Tejaswi Ravikumar Chitrapu, Xin Chen, Siu-Wai Chan.

4:40 PM - 5:00 PM
Polymorphism and its influence on metathesis reactions. Rebecca McAuliffe, Rebecca McAuliffe, Paul Todd, James Neilson, Gabriel Veith.

4.2.5: Sustaining Crystallography Education and Training
Supporting SIGS: General Interest, Service Crystallography
Presented With Support from Bruker
Session Start Time: 01:30 PM | Room: Ballroom C
Chair(s): Joe Tanski, Brian Toby

1:30 PM – 1:40 PM Introduction

1:40 PM - 2:00 PM
Incorporating Crystallography into a Short-Term Research Experience. Dean Johnston.

2:00 PM - 2:20 PM
Building the future of crystallography though active engagement. Suzanna Ward, Amy Sarjeant.

2:20 PM - 2:40 PM
Undergraduates, Crystals, and Crystallography
Lauren DePue, Richard Jones, Emily Que, Andrew Kalamarides, Lauren Ohman, Reem Al-Sayyad, Areefa. Rahman, Brandon O'Neal.

2:40 PM - 3:00 PM
Embracing Student-Centered Guest Lectures in Crystallography Education for Chemistry Students. Shao-Liang Zheng.

3:00 PM – 3:30 PM Coffee Break

3:30 PM - 3:50 PM
The Rigaku XtaLAB Mini for use across the undergraduate curriculum to teach single crystal x-ray crystallography. Sandy Eagle, Reza Mohseni.

3:50 PM - 4:10 PM
3D printing of molecular models to support undergraduate and graduate teaching and research. Marvin Hackert.

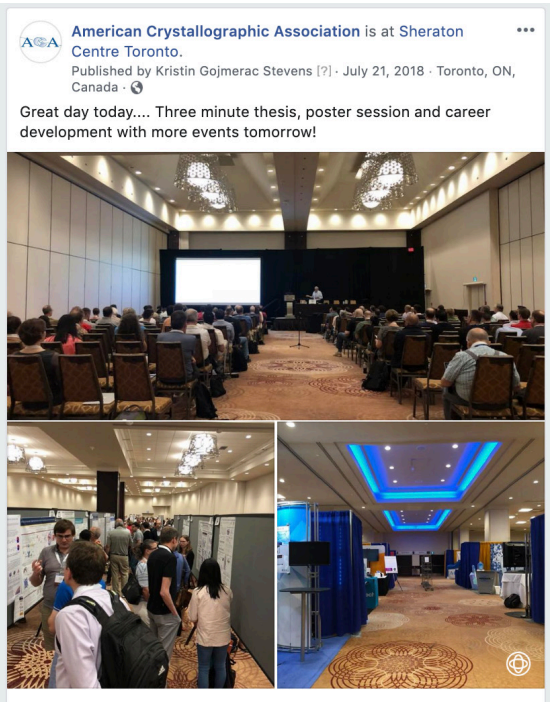
4:10 PM - 4:30 PM
Hooked on crystallography. Michael Ruf, Bruce Noll.

4:30 PM - 4:40 PM
Doing Structural Coordination Chemistry Research with Limited Funds. Mark Whitener.

Let's Get Social....

Like, share and tag the ACA on Facebook:

www.facebook.com/AmerCrystalAssn/



Like, share and tag on Twitter:

@ACAxtal
#aca2019mtg
#crystallography
#crystallographersarecool

POSTER INFORMATION

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 $100 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.

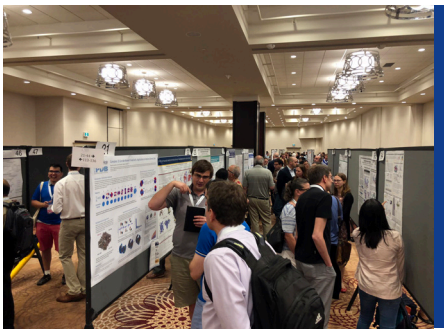
Oxford Cryosystems Low
Temperature Poster Prize
This prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.

Journal of Chemical
Crystallography Poster Prize
The best gradudate 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 Sunday, July 21, until 7:30 pm on Monday, July 23. Please be present at your poster from 5:30 - 7:30 pm on the day to which you are assigned. Posters beginning with PS1 present on Sunday. Posters beginning with PS2 present on Monday. Poster beginning with PS3 present on Tuesday.



POSTER SESSIONS:

Poster Session 1: Sunday, July 21, 2019 [5:30 PM - 7:30 PM]

Poster Session 2: Monday, July 22, 2019 [5:30 PM - 7:30 PM]

Poster Session 3: Tuesday, July 23, 2019 [5:30 PM - 7:30 PM]

PS1–1 Solving structures by native SAD at room temperature
Förster, Andreas

PS1–2 Structural Basis of Tubulin Recruitment and Assembly by Microtubule Polymerases
Nithianantham, Stanley

PS1–3 Scalable Synthesis of a Cyclobutane-1, 2-diacid Building Block from trans-Cinnamic Acid via Photoreaction
Amjaour, Houssein

PS1–4 Co-crystal structure of Protein kinase C-iota with inhibitor reveals an unique binding mode
Baburajendran, Nithya

PS1–5 Crystallographic Study of Dihydroneopterin Aldolase from Helicobacter pylori
Shaw, Gary

PS1–6 Structures of TAPBPR/MHC-I and TAPBPR/nanobody complexes; rigidification of dynamic regions on interaction with ligands
Jiang, Jiansheng

PS1–7 Tuned Effector Functions and Adduct Structures of an Engineered Human Fc Fragment
Gallagher, Travis

PS1–8 Biochemical and Structural Investigation of the Dynamic Regulation Mechanism of Pyruvate Kinase Muscle Isoform 2 using Amino Acids
Nandi, Suparno

PS1–9 The structure of IL-11 Mutein suggests a surprising mechanism of inhibition
Metcalfe, Riley

PS1–10 Background Modelling in transmission X-Ray Powder Diffraction (XRPD) of Pharmaceutical Compounds: a comparative analysis of different approaches
Ramirez, Barbara

PS1–11 Structural and mechanistic basis for CBP/P300 recruitment to the Notch transcription complex
Kolb, Ellie

PS1–12 Elucidation of the Photoreactivity of nanocrystalline 2-hydroxychalcones using continuous flow method
George, Sobiya

PS1–13 The small-angle X-ray scattering core facility of center for cancer research of National Cancer Institute
Fan, Lixin

PS1–14 A protein crystallization strategy for structure-based drug design
Bergfors, Terese

PS1–15 Structures of ClpC1-NTD with potent anti-TB cyclic peptides Rufomycin and Ecumicin: Implications for the mechanism of action and design of therapeutic agents
Wolf, Nina

PS1–16 Structural Interrogation of Proteins Involved in the Biosynthesis of 10-Membered Enediyne Anticancer Natural Products
Kosgei, Abigael

PS1–17 Engineering slow acting mono-Zn variants of metallo β-lactamases as a crystallographic and spectroscopic platforms for drug discovery
Page, Richard

PS1–18 Structures of Lsm rings from S. pombe
Montemayor, Eric

PS1–19 Structural basis of FbpA-mediated periplasmic iron transport in Moraxella catarrhalis
Chan, Clement

PS1–20 Exploring Low-Energy Pathways that Interconvert the Apo and Bound States of a Metabolite-Sensing Gene-Regulatory RNA Switch
Wedekind, Joseph

PS1–21 Structural Insights into UBAN-PolyUbs Assembly
LO, YU-CHIH

PS1–22 Evolution of a Bifunctional Reductase/Diels-Alderase for Fungal Indole Alkaloid Biosynthesis
Dan, Qingyun

PS1–23 Crystallization of an Archaeal Dihydroorotase
Vitali, Jacqueline

PS1–24 Contact-dependent growth inhibition tRNase toxin-immunity protein complexes from Escherichia coli 3006 and Klebsiella pneumoniae 342
Michalska, Karolina

PS1–25 Next-Generation Home-Lab Systems for the Changing Structural Biology Landscape
Benning, Matthew

POSTER INFORMATION [Sunday]

PS1−26 ZBTB24 regulates gene transcription by recognizing the core promoter of CDCA7
ren, ren

PS1−27 Structural basis of SETD3 as an actin histidine methyltransferase
Dai, Shaobo

PS1−28 Structural basis for preferential binding of human TCF4 to DNA containing 5-carboxylcytosine
yang, jie

PS1−29 Updated Validation and Deposition Tools in the Phenix GUI
Poon, Billy

PS1−30 ACT domain of Bacillus anthracis prephenate dehydrogenase acts as tyrosine sensor and inhibits the enzyme via a mechanical switch
Shabalin, Ivan

PS1−31 Mixed-linkage ubiquitin chains as complex regulators of cellular signaling pathways
Rahighi, Simin

PS1−32 Structural Insights into Catalytic Versatility of the Flavin-dependent Hydroxylase (HpaB) from Escherichia coli
Rose, John

PS1−33 Symmetry Analysis of the Toroidal Moment in Magnetoelectric Crystalline Materials
Gnewuch, Stephanie

PS1−34 Structural studies of a novel ubiquitin-modifying enzyme, SdeA using various tools
Kim, Leehyeon

PS1−35 Structural studies on low-dose X-ray radiation induced Transforming growth factor beta-1 (TGFβ-1) activation
Stachowski, Timothy

PS1−36 Furan-2,5-dicarboxylic acid, a promising platform molecule: polymer, monomer, and MOF
Mao, Yimin

PS1−37 Hydrogen Bonding in High-Z' Molecular Structures
Carta, Veronica

PS1−38 Structural analysis shows spliceosome-induced closure of an alpha-helical super-helix in the proto-oncogenic splicing factor SF3b1
Maji, Debanjana

PS1−39 Neutron Diffraction Studies of PLP-Dependent Enzymes
Drago, Victoria

PS1−40 Structural Characterization of Lab-Evolved Proteins Reveals Signature Sequences Required for High-Affinity Binding to HIV-1 TAR RNA
Chavali, Sai Shashank

PS1−41 Crystallographic analysis of tryptophan halogenases AbeH and BorH
Ashaduzzaman, Md

PS1−42 Attempts and approximations for a background modeling in pharmaceutical samples in patterns of XRD and S-XRPD
Ramirez, Barbara

PS1−43 X-ray Crystal Structure Determination of LTA4H:4MDM:PGP Analogue Complex and Characterization of the Aminopeptidase Enzyme Mechanism
Lee, Kyung Hyeon

PS1−44 Identifying the effects of N-glycan differences between Nicotiana benthamiana and Pichia pastoris on recombinant enzymes
Fraser, Nicole

PS1−45 Towards the Architecture of the TOC Protein Complex
Srinivasan, Karthik

PS1−46 A Conserved PLPLRT/SD Motif within the C-terminal Tail of STING Mediates the Recruitment and Activation of TBK1
u, Pengbiao

PS1−47 A database of high-quality protein residues for reference data, library construction, and motif analysis
Williams, Christopher

PS1−48 Determining the reactivity of photodynamic crystals of o-azidostilbene
Patton, Leanna

PS1−49 MD-assisted refinement of x-ray coordinates
Mikhailovskii, Oleg

PS2−1 Characterization of the β-barrel Assembly Machinery in Nanodiscs using Cryo-EM
Wu, Runrun

PS2−2 Micro Electron Diffraction is a quick and versatile tool for structure determination of macromolecules and small molecules
Yakushevska, Alevtyna

PS2−3 chameleon: Next Generation Sample Preparation for CryoEM based on Spotiton
Browning, Dawn

PS2−4 Local structural study of novel mott-insulating cousins of the iron pnictides
Karki, Bhupendra

PS2−5 Crystal Structure Reveals a Unique ABIN-Ubs Binding Mode
Hong, Jhen-Yi

PS2−6 Investigating the interaction of EtpA and flagellin from enterotoxigenic Escherichia coli (ETEC)
Ntui, Clifford Manyo

PS2−7 Myxobacterial phytochromes as light-regulated enzymes suitable for XFEL studies
Stojkovic, Emina

PS2−8 Analysis of differences in crystal movements from gas releasing crystals as dictated by lattice energy interactions
Shields, Dylan

PS2−9 Photoinduced self-stirring crystals caused by gas release
Banerjee, Upasana

PS2−10 Linkage of crystal lattice and photodynamic behavior of organic crystals
Abdelaziz, Nayera

PS2−11 The crystal structure and slow time-resolved oxidative decay of an E. coli DHFR complex with tetrahydrofolate with implications to drug design
Cao, Hongnan

PS2−12 Using a supercomputer for massive parallel merging of XFEL reflections
Bolotovsky, Robert

PS2−13 Processing data from new XFELs in cctbx.xfel and DIALS
Brewster, Aaron

PS2−14 Applications of a New Program for the Reconstruction of Protein Envelopes from Solution Scattering Data
Badger, John

PS2−15 SAXS and X-ray crystallographic studies of the assembly of the CARD promoter of the apoptosome
Lin, Su-Chang

PS2−16 A Supramolecular Synthon Containing Two Five-coordinate (Octaethylporphinato)Iron(III) Hemes
Haller, Jeffrey

PS2−17 Supramolecular Analysis of a Multi-Cation Hydrated Decavandate Salt
Haller, Joseph

PS2−18 A supramolecular toolkit for structure determination
Li, Yuantao

PS2−19 Non-negative matrix factorization for isolating damage-free reflections in macromolecular synchrotron data collection
Sarkar, Sreya

PS2−20 Dynamic Sampling for Minimizing Crystal Damage Prior to Diffraction Data Collection
Simpson, Garth

PS2−21 Radiation decay of thaumatin crystals at three X-ray energies
Rosenbaum, Gerold

PS2−22 Structural characterization of capillary morphogenesis gene 2 inhibitors
Soleimani, Sara

PS2−23 Probing the thermal stability and X-ray crystal structures of select members of the Verona integron-encoded metallo-β-lactamase 2 family
Page, Richard

PS2−24 Atomic structure of nanomaterials by resonant high-energy XRD
Petkov, Valeri

PS2−25 Local Structure Investigation of Rapidly Synthesized WxV1-xO2
Wilson, Catrina

POSTER INFORMATION [Monday]

PS2−26 Remote Access Synchrotron: Small Molecule collection on Macro-instrument: An Analysis of the software for integration.
Staples, Richard

PS2−27 New polymorphs of isoniazid: discovery from melt experiments
zhang, keke

PS2−28 Synthesis of Cu and Co complexes of bosentan and study of solubility at different pHs
Henao, JOSE ANTONIO

PS2−29 Migrating the fast_dp software package for Python 2 and 3 compatibility
Bernstein, Herbert J.

PS2−30 Structure analysis of transcription related complexes and installation of cryo-EM in KEK
Adachi, Naruhiko

PS2−31 NIH Transformative High Resolution Cryo-Electron Microscopy Program
Wu, Mary Ann

PS2−32 The structure of the Plasmodium falciparum 20S proteasome in complex with the PA28 activator.
Metcalfe, Riley

PS2−33 An update on detergent usage in cryo-EM structure determination of membrane proteins
Pryor, Edward

PS2−34 Z-contrast enhancement for small protein cryo-EM structure determination
Chen, James

PS2−35 A capillary device for growing large protein crystals
Inaka, Koji

PS2−36 Relating crystal structure to vapochromic responses in polymorphic compounds
Barker, Nathaniel

PS2−37 Acidic substrate tunnel redesign by loop transplant to enhance SES7 selectivity towards base amino acids
tang, heng

PS2−38 Exploring the Hydrogen Bond Enhanced Halogen Bond
Decato, Daniel

PS2−39 Polymorphic transformations of [Co(μ-OOCtBu)2py]2
Wheaton, Amelia

PS2−40 Improving understanding of RNA structures with the PHENIX/AMBER interface
Gray, Jonathon

PS2−41 Probing Open Metal Sites in High Valence Metal-Organic Frameworks by in-situ Single Crystal X-ray Diffraction
Wang, Qi

PS2−42 Effects of zinc ion on oligomerization and pH stability of influenza virus hemagglutinin
Seok, Jong Hyeon

PS2−43 Steric Effects Associated with the Photolysis of [Ru(biq)2(dpb)](PF6)2 and [Rb(biq)2(CH3CN)2](PF6)2
Lake, Charles

PS2−44 Structure of the WFIKKN2 Follistatin domain and insight into GDF8 and GDF11 antagonism
McCoy, Jason

PS2−45 Exploring the Crystal Structure and Functional Role of the Lectin Domain from the Staphylococcal Biofilm Protein Aap
Maciag, Joseph

PS2−46 Photoreactivity of β, γ, ε-alkyl azide derivatives in crystals
Merugu, Rajkumar

PS2−47 Crystallization of two alpha-glucosidases found in Bacteroides thetaiotaomicron
Reid, Clarisse

PS3−1 Mechanistic Insights into the Superexchange-Interaction-Driven Negative Thermal Expansion in CuO
Zhang, Yuanpeng

PS3−2 The death of powder – micro-electron diffraction with EIGER
Schulze-Briese, Clemens

PS3−3 NMR Crystallography Advancements for Exploring Polymorphism
Baias, Maria

PS3−4 MetalJet source for x- ray scattering and diffraction studies
Adibhatla, Anasuya

PS3−5 The latest update of the Advanced Crystallography program at NSF's ChemMatCARS
Wang, SuYin

PS3−6 Macromolecular Crystallography at MAX IV
Gonzalez, Ana

PS3−7 New capabilities at beamline 11-ID-B of the Advanced Photon Source
Borkiewicz, Olaf

PS3−8 Update from the Life Science X-ray Scattering (LiX) beamline at NSLS-II
Yang, Lin

PS3−9 Beamline operating software B4 and automated crystallography suite at the Berkeley Center for Structural Biology
Allaire, Marc

PS3−10 Obtaining Anisotropic Atomic Displacements from NMR Methods
Harper, James

PS3−11 Locating H atoms: active site protomer/tautomer state determination using routine, macromolecular X-ray diffraction and BUSTER/DivCon
Borbulevych, Oleg

PS3−12 Color-Coding Point Group and Space Group Diagrams
Slebodnick, Carla

PS3−13 Structure of a Self-Assembled Three-Dimensional DNA Crystal Framework for the Precise Organization of Biomaterials
Simmons, Chad

PS3−14 The Rigaku Oxford Diffraction XtaLAB Synergy: from Powder Analysis to Charge Density Studies and Protein Structure Solution.
Le Magueres, Pierre

PS3−15 An EPR and Crystallographic Investigation of Copper-doped Cadmium Creatinine Sulfate
Vitali, Jacqueline

PS3−16 Autoscoring of Protein Crystallization Drops in ROCK MAKER using MARCO
Ramsey, Lance

PS3−17 Volumetric and hygrometric performance of the NT8®, an advanced liquid handler for high throughput crystallization screening
Ramsey, Lance

PS3−18 Practical aspects of sample concentration and buffer exchange utilizing a miniaturized tangential flow filtration (TFF) system
Logan, Baker

PS3−19 SASE-MAD protein structure determination and charge assignment to metal sites using XFEL crystallography
Bhowmick, Asmit

PS3−20 Consideration of improved data accuracy in solvent removal and crystal processing using the deep UV laser
Harada, Ayaka

PS3−21 SANS contrast applied to study hierarchical structure of plant biomass during assembly and deconstruction
Pingali, Sai Venkatesh

PS3−22 Empirical lead generation by crystallographic screening of fragment libraries
Das, Debanu

PS3−23 In situ synchrotron investigations in large volume presses at high pressure and high temperature
Lathe, Christian

PS3−24 Structural analysis by stochastic differential scanning calorimetry
Sherman, Alex

PS3−25 Exploring the SPARK of Science with a New Light
Perez, Aleida

POSTER INFORMATION [Tuesday]

PS3−26 From Art to Science: Advanced Cryocooling Technology for Biomolecular Cryocrystallography
Apker, Benjamin

PS3−27 Visualizing the long non-coding subgenomic flavivirus RNAs in solution
Fang, Xianyang

PS3−28 SEC-SAXS on an in-house laboratory instrument
Skou, Soren

PS3−29 Time-Resolved Solution Scattering for Structural Biology Research at SSRL BL4-2
Wiess, Thomas

PS3−30 Characterizing macromolecular samples using SAXS and WAXS
Criswell, Angela

PS3−31 Enabling Depositor-initiated PDB coordinate replacement through file versioning
Zardecki, Christine

PS3−32 Faster, Simpler Bravais Lattice Determination in S6
Andrews, Lawrence

PS3−33 Data Analysis for Synchrotron Microcrystal Native-SAD Phasing
Liu, Qun

PS3−34 NE-CAT: Crystallography Beamlines for Challenging Structural Biology Research
Banerjee, Surajit

PS3−35 Exploring Biology and Medicine Using 3D Biomacromolecules with PDB-101
Zardecki, Christine

PS3−36 Recent developments in Bio-SAXS using MetalJet X-ray source
Adibhatla, Anasuya

PS3−37 Utilizing engineered nucleation features to increase productivity in protein crystallization trials
Kinnibrugh, Tiffany

PS3−38 Electron Density Distributions in 2-(dimethylamino)biphenyl-2'-carboxaldehydes
Martin, Kenneth

PS3−39 Use of enhanced nucleation surfaces in a continuous flow crystallization system
Nordquist, Kyle

PS3−40 The essential pre-mRNA splicing factor U2AF65 accommodates divergent nucleotides at the central position of the polypyrimidine 3´ splice site signal
Glasser, Eliezra

PS3−41 Protein and Crystallography Facility at the University of Iowa
Xu, Zhen

PS3−42 Examples of the direct phasing of protein structures with high solvent contents
Miller, Mitchell

PS3−43 How to Remedy Incorrect Duplicates in the CSD?
Fronczek, Frank

PS3−44 Relating Nanostructure to Macroscopic Properties Using A Laboratory Rheo-SAXS Setup
Keilbach, Andreas

PS3−45 Integrating SAXS and Complementary Techniques for Structure Determination of Biomolecules
Keilbach, Andreas

PS3−46 Strong translational NCS leads to space group ambiguity or how close inspection of data can rescue structures. Two examples from SSGCID
Abendroth, Jan

PS3−47 Thermo Fisher Scientific -
Lau, Cristina

PS3−48 Improvements in Serial Crystallography Capabilities at GM/CA
Kissick, David

PS3−49 How new strategies can improve productivity - rMMS microseeding for crystallization and DLS for cryoEM
Patrick Stewart, Douglas

PRESENTING AUTHOR INDEX

PRESENTING AUTHOR INDEX

PRESENTING AUTHOR INDEX

ACA MEETING CODE OF CONDUCT

[Wording of this policy generously provided by American Geophysical Union]

The ACA Meeting is an annual event providing scientists from a wide variety of backgrounds the opportunity to exchange cutting edge ideas and techniques in multiple areas of research. Each meeting highlights various aspects of crystallography and demonstrates their significance to the greater scientific community. ACA is committed to providing a safe, productive, and welcoming environment for all meeting participants and ACA staff. All participants, including, but not limited to, attendees, speakers, volunteers, exhibitors, ACA staff, service providers and others are expected to abide by this ACA Meetings Code of Conduct. This Code of Conduct applies to all ACA meetings and meeting related events, including those sponsored by organizations other than ACA but held in conjunction with ACA events, in public or private facilities.

This code of conduct will be in force after ratification by the Council of the ACA on the 24th day of March 2016:

Expected Behavior

All participants, attendees, ACA staff, and vendors should treat each other with respect and consideration, valuing a diversity of views and opinions.

They should be considerate, respectful, and collaborative with others.

They should communicate openly with respect for others, critiquing ideas rather than individuals.

They should avoid personal attacks directed toward other attendees, participants, ACA staff, and suppliers/vendors.

They should be mindful of their surroundings and their fellow participants. ACA staff should be alerted if you notice a dangerous situation or someone in distress.

They should respect the rules and policies of the meeting venue, hotels, ACA contracted facility, or any other venue.

Unacceptable Behavior

Harassment, intimidation, or discrimination in any form will not be tolerated.

Physical or verbal abuse of any attendee, speaker, volunteer, exhibitor, ACA staff member, service provider, or other meeting guest will not be tolerated.

Examples of unacceptable behavior include, but are not limited to, verbal comments related to gender, sexual orientation, disability, physical appearance, body size, race, religion, national origin, inappropriate use of nudity and/or sexual images in public spaces or in presentations, or threatening or stalking any attendee, speaker, volunteer, exhibitor, ACA staff member, service provider, or other meeting guest.

Recording or taking photography of another individual's presentation without the explicit permission of ACA is not allowed.

Disruption of talks at oral or poster sessions, in the exhibit hall, or at other events organized by ACA at the meeting venue, hotels, or other ACA contracted facilities.

Consequences

Anyone requested to cease unacceptable behavior will be expected to comply immediately.

ACA staff (or their designee) or security may take any action deemed necessary and appropriate, including immediate removal from the meeting or the conference without warning or refund.

ACA reserves the right to prohibit attendance by anyone violating this code of conduct at any future meeting.

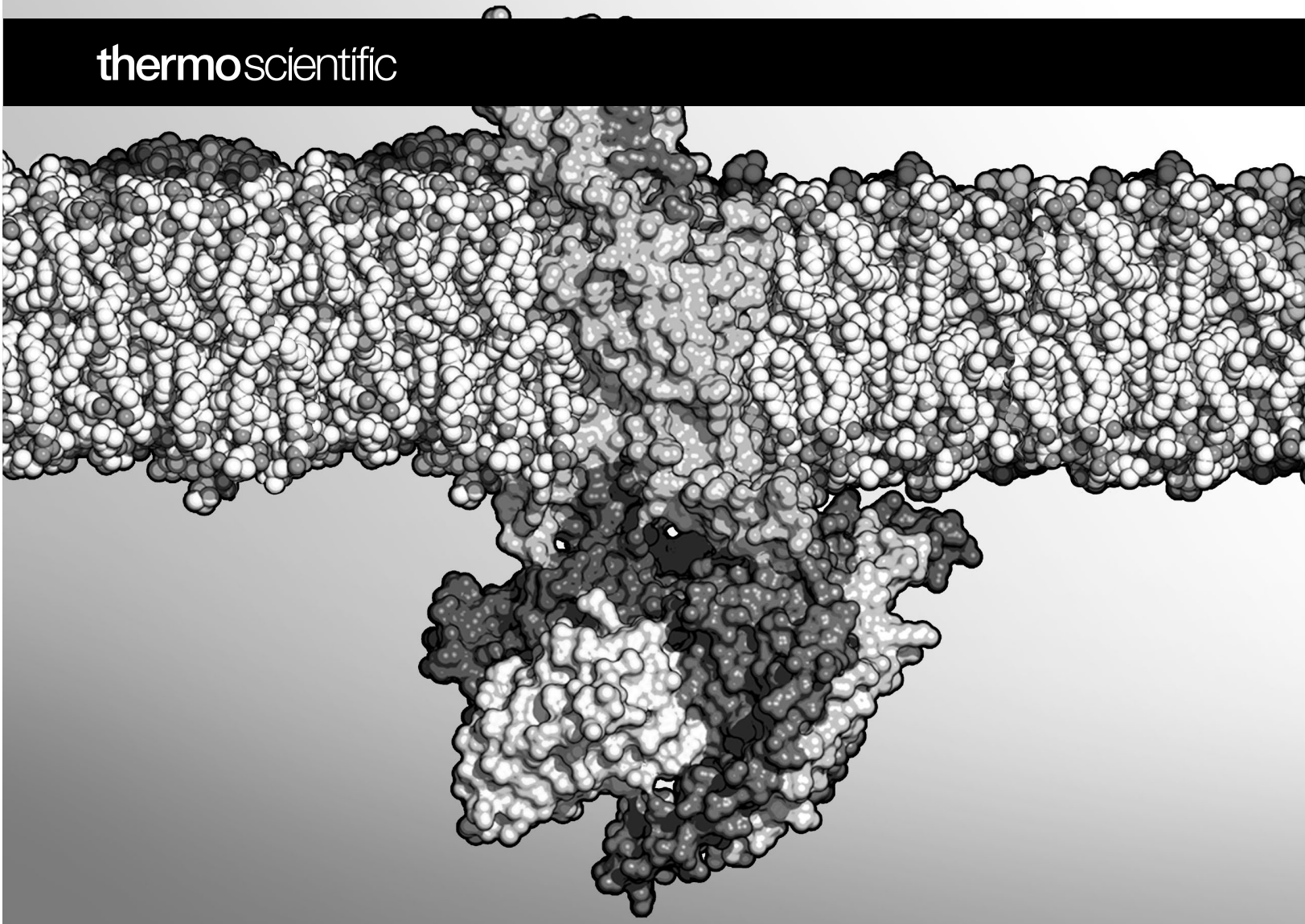
For repeated or flagrant violations membership in ACA may be cancelled or suspended by action of a majority of the executive board.

Reporting Unacceptable Behavior

If you are the subject of unacceptable behavior or have witnessed any such behavior, please immediately notify an ACA staff member or ACA volunteer in a leadership position. Notification should be done by contacting an ACA staff person on site or by emailing your concern to aca@hwi.buffalo.edu.

Anyone experiencing or witnessing behavior that constitutes an immediate or serious threat to public safety is advised to contact 911 and locate a hotel house phone and ask for security.

thermoscientific



Your partner in science

Our experts in booth **201** have the details on all the challenges to engaging in cryo-electron microscopy. Discover the support Thermo Fisher Scientific provides to minimize these challenges so you can integrate our solutions into your workflow.

Also learn about an exciting micro electron diffraction technique for fast and high resolution 3D structure determination of small chemical compounds and biological macromolecules.

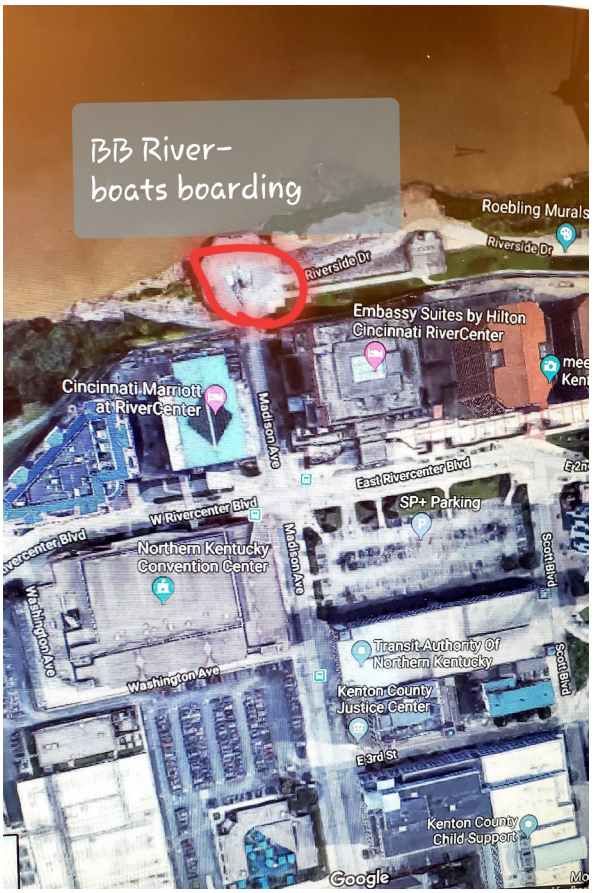
Find out more at
cryo-electronmicroscopy.com
thermofisher.com/MicroED

ThermoFisher
SCIENTIFIC

CLOSING BANQUET

Wednesday, 7/24/2019 @ 6:30 PM
Belle of Cincinnati

While traditionally held onsite, in 2019 the ACA closing banquet will be held offsite on the Belle of Cincinnati on Wednesday, July 24, 2018, in the evening. Join us, just a short walk from the hotels, on the Belle of Cincinnati for a banquet dinner reception (buffet), cash bar, and networking with fellow attendees.



Boarding Time: 6:00 PM
Sailing Time: 7:00 PM
Docking Time: 9:00 PM

Please join us at the BB Riverboats Boarding dock just a short walk from either hotel (above). Boarding will begin promptly at 6:00 PM and the boat will sail at 7:00 PM returning to the dock for the evening at 9:00 PM and continuing the party at the dock with music from the Trailer Park Floosies!

2020 PLANNING MEETING

Thursday 7/25/2019 @ 8:00 AM
NKCC
Meeting Rooms 9-10 (MR910)

SAVE THE DATES!

SATURDAY, AUGUST 1-THURSDAY, AUGUST 6, 2020

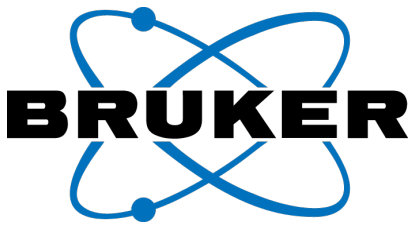
Sheraton San Diego Hotel & Marina

July 30 - August 3, 2021
Baltimore Marriott Waterfront

July 29 - August 2, 2022
Portland Marriott Downtown Waterfront

VENDOR PASSPORT

This year select vendors are participating in a Vendor Passport contest. To be eligible for the $50 drawings, please complete all stops on the passport below and collect stamps from each participant. Once complete, tear and return to the registration desk with your contact information below, on or before noon on July 23, 2019. The drawing will be held at the final poster session 6:00 P.M. on July 23, 2019.



NAME: _____

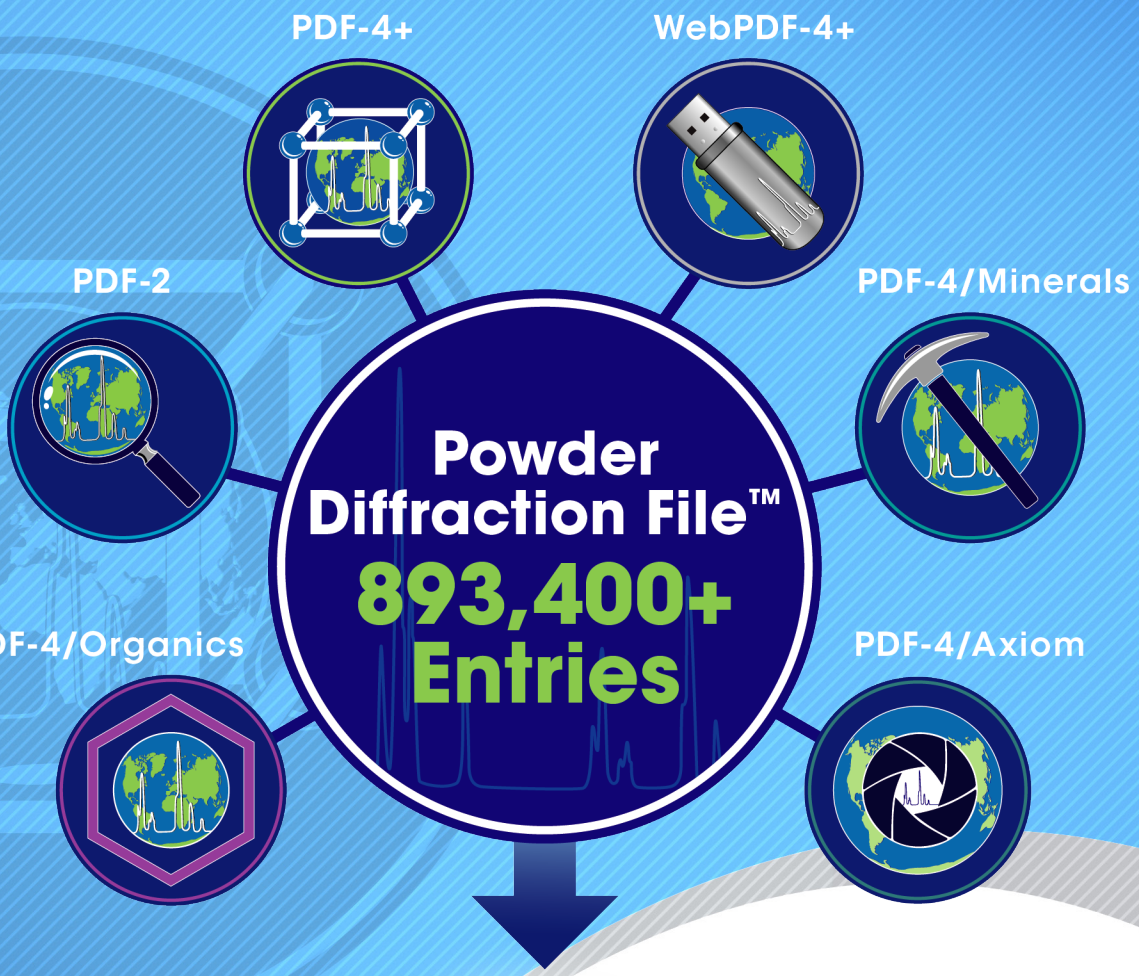
EMAIL: _____

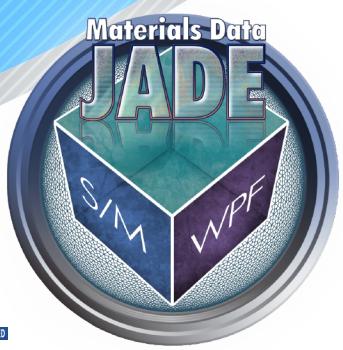
TELEPHONE NUMBER: _____

INTERNATIONAL CENTRE FOR DIFFRACTION DATA

Diffraction Data You Can Trust

ICDD databases are the only crystallographic databases in the world with quality marks and quality review processes that are ISO certified.





ISO 9001:2015 QUALITY MANAGEMENT SYSTEM CERTIFIED BY DEKRA CERT. NO. 110409.01

ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

MDI
Materials Data™

Visit us at ACA Booth #312

www.icdd.com | marketing@icdd.com

AT A GLANCE

	TIME	ROOM	TITLE	TIME	ROOM	TITLE	TIME	ROOM	TITLE
FRI							4:00PM	MR10	Bystander Training (Invite Only)
FRI							6:00 PM	1STLOB	Registration Reception
SAT	8:00 AM	MR1	Workshop #3 – AM SESSION	1:30 PM	MR1	Workshop #3 – PM SESSION	5:30 PM	MR5	First Time Attendee & Student Orientation
SAT	8:30 AM	MR2	Workshop #4 – AM SESSION	1:30 PM	MR2	Workshop #4 – PM SESSION	6:30 PM	BR-B	Keynote Session: Michael G. Rossmann Memorial Lecture
SAT	8:30 AM	MR3	Workshop #6 – AM SESSION	1:30 PM	MR3	Workshop #6 – PM SESSION	7:30 PM	HALL1	Exhibit Show & Reception
SAT	8:30 AM	MR5	Workshop #1 – AM SESSION	1:30 PM	MR5	Workshop #1 – PM SESSION			
SAT				1:00 PM	MR6-7	Workshop #2 – PM SESSION			
SUN	8:00 AM	BR-B	PL1 Trueblood Award: Brian Toby & Robert Von Dreele	12:00 PM	BR-B	Three Minute Thesis A	5:00 PM	BR-B	Canadian Division SIG
SUN	9:00 AM	LRNCNT	T1 Transactions—Data Best Practices: Current State and Future Needs	12:00 PM	BR-C	Three Minute Thesis B	5:30 PM	HALL1	Poster Session
SUN	9:00 AM	BR-B	1.1.1 Macromolecular Structure Under Physiological Conditions	12:00 PM	LRNCNT	Best Practices SIG			
SUN	9:00 AM	BR-D	1.1.2 Cutting Edge Studies using Cryo Electron Microscopes	12:00 PM	BR-D	Cryo-EM SIG			
SUN	9:00 AM	BR-C	1.1.3 Morphological Characterization of Porous Materials	12:00 PM	MR6	Fiber SIG			
SUN	9:00 AM	BR-E	1.1.4 Crystallography in the Geosciences	12:00 PM	BR-E	Small Angle Scattering SIG			
SUN				1:15 PM	LRNCNT	T2 Transactions—Data Best Practices: Current State and Future Needs			
SUN				1:30 PM	BR-B	1.2.1 Structure Without Structure [Structural Dynamics Session]			
SUN				1:30 PM	BR-D	1.2.2 Crystallography at Extreme Conditions			
SUN				1:30 PM	BR-C	1.2.3 Understanding Polymer Structure and Dynamics During and After Processing			
SUN				1:30 PM	BR-E	1.2.4 Magnetic, Quantum, and Electronic Correlated Materials			
MON	8:00 AM	BR-B	PL2 Fankuchen Award: Eaton (Ed) Lattman	12:00 PM	BR-D	Three Minute Thesis FINALS!	5:00 PM	LRNCNT	BioMac SIG
MON	9:00 AM	BR-B	2.1.1 Structure in Cancer Biology I	12:00 PM	MR2-3	Dectris Lunch & Learn	5:00 PM	MR7	Industrial SIG
MON	9:00 AM	BR-E	2.1.2 Microcrystal Electron Diffraction	12:00 PM	LRNCNT	General Interest SIG	5:00 PM	BR-C	[JOINT SIG MTG] Materials Science, Neutron Scattering & Powder Diffraction
MON	9:00 AM	BR-C	2.1.3 Diffuse Scattering for Biological Structure and Dynamics	12:00 PM	MR7	Light Sources SIG	5:30 PM	HALL1	Poster Session
MON	9:00 AM	BR-D	2.1.4 Solid State NMR Crystallography	12:00 PM	BR-C	[JOINT SIG MTG] Service Crystallography & Small Molecules	6:00 PM	MR1	Fellows Reception [Invite Only]
MON	9:00 AM	MR7	2.1.5 Crystal Structure Solution from Powder Data	12:00 PM	BR-B	Young Scientists	7:00 PM	MR3	CCDC Mixer
MON	9:00 AM	LRNCNT	2.1.6 What is a Crystal, In Time & Space	1:30 PM	MR7	2.2.1 Powder Diffraction in Industry	8:00 PM	OFFSITE The Loft Braxton Brewing	YSIG Mixer
MON				1:30 PM	BR-C	2.2.2 New Toys: Sources, Beamlines and Detectors			
MON				1:30 PM	BR-D	2.2.3 Locating and Refining H Atoms Using X-rays, Neutrons, and Solid-State NMR			
MON				1:30 PM	BR-B	2.2.4 General Interest I			
MON				1:30 PM	LRNCNT	2.2.5 Crystallization on the International Space Station			
				1:30 PM	BR-E	WK5A Cryo-EM Workshop I: Image Processing			
TUES	8:00 AM	BR-B	PL3 Bau Award: Bryan Chakoumakos	1:30 PM	LRNCNT	3.2.1 Application of Anomalous Techniques in Macromolecular Crystallography	5:00 PM	LRNCNT	3.3.1 Would You Publish This?
TUES	9:00 AM	LRNCNT	3.1.1 Structure in Cancer Biology II	1:30 PM	BR-C	3.2.2 SAS Contrast Methods in Biology and Soft Matter	5:00 PM	BR-B	All Members Business Meeting
TUES	9:00 AM	BR-C	3.1.2 Time Resolved Macromolecular Structure Determination at X-ray Free Electron Lasers	1:30 PM	BR-D	3.2.3 Home-Built Software and Hardware	5:30 PM	HALL1	Poster Session
TUES	9:00 AM	BR-D	3.1.3 Structural Biology Combining Solution SAS and High Resolution Methods (cryoEM, MX, NMR)	1:30 PM	BR-B	3.2.4 Solid State Supramolecular Chemistry and Crystal Engineering Part II			
TUES	9:00 AM	BR-B	3.1.4 Solid State Supramolecular Chemistry and Crystal Engineering Part I	1:30 PM	BR-E	WK5B Cryo-EM Workshop II: Reconstruction*			
TUES	9:00 AM	BR-E	3.1.5 Functional Sustainable Materials						
WED	8:00 AM	BR-B	PL4 Margaret C. Etter Early Career Award: Efrain Rodriguez	1:30 PM	BR-D	4.2.1 What is the Meaning of Resolution?	6:00 PM	OFFSITE: Belle of Cincinnati	Banquet
WED	9:00 AM	BR-B	4.1.1 Central Dogma in 3D: The Legacy of Tom Steitz	1:30 PM	LRNCNT	4.2.2 Structure Based Drug Design			
WED	9:00 AM	BR-D	4.1.2 Radiation Damage in X-ray Crystallography and Cryo-EM	1:30 PM	BR-B	4.2.3 Cool Structures: Important Science from Small Molecule Crystallography			
WED	9:00 AM	LRNCNT	4.1.3 Cool Structures: Important Science from Small Molecule Crystallography	1:30 PM	BR-E	4.2.4 In situ and Operando Measurements			
WED	9:00 AM	MR7	4.1.4 In situ and Operando Characterization of Functional Films	1:30 PM	BR-C	4.2.5 Sustaining Crystallography Education and Training			
WED	9:00 AM	BR-C	4.1.5 Diversity & Inclusion -- Diverse Teams Perform Better						
WED	9:00 AM	BR-E	4.1.6 General Interest II						
WED	8:00 AM	MR9-10	2020 Planning Meeting						

EXHIBIT SHOW HOURS

Saturday, July 20, 2019 7:30 PM - 10:30 PM OPENING RECEPTION!

Sunday, July 21, 2019 10:00 AM - 12:00 PM | Closed for Lunch from 12:00 PM - 2:00 PM | Sunday, July 21, 2019 2:00 PM - 7:30 PM

Monday, July 22, 2019 10:00 AM - 12:00 PM | Closed for Lunch from 12:00 PM - 2:00 PM | Monday, July 22, 2019 2:00 PM - 7:30 PM

Tuesday, July 23, 2019 10:00 AM - 12:00 PM | Closed for Lunch from 12:00 PM - 2:00 PM | Tuesday, July 23, 2019 2:00 PM - 7:30 PM