2024

2024 ACA Annual Meeting Summary

ACA: The Structural Science Society
https://www.amercrystalassn.org/
2024 Full Program with Abstract List

Contents

Badge Pickup

7:00 - 8:00pm Saturday, 6th July, 2024
Rocky Foyer - Pint Brothers BY

If you arrive early on Saturday, we encourage you to stop by and pick up your conference badge ahead of time. Our registration desk will be open for an hour in the evening providing you with a convenient opportunity to avoid the rush. We look forward to welcoming you and ensuring you have a smooth and enjoyable experience at ACA2024.

Registration Desk

7:00am - 6:00pm Sunday, 7th July, 2024
Rocky Foyer - Pint Brothers BY

WK2: Applications of Small Angle Scattering to Structural Biology: An Introduction

8:00am - 5:30pm Sunday, 7th July, 2024
Evergreen D
Jesse Hopkins, Michal Hammel

Small angle X-ray and neutron scattering (SAXS/SANS, or SAS) has experienced dramatic growth within the structural biology community over the past fifteen years, emerging as an important and versatile analytical technique for the study of the structure and function of biological macromolecules in solution. This workshop will introduce both the theory of the method and best practices common to the field and will include lectures and a selection of hands-on practical exercises. Throughout the workshop the emphasis will be on practical application: knowing how to judge data quality, how to troubleshoot during data collection, and the expectations for a successful experiment and acceptable publication. Students will also learn about aspects of home laboratory data collection and important complementary biophysical techniques for validating your SAS data.

Workshop topics include:

-Basic principles of SAS

-Critical sample preparation and data collection procedures, including SEC-SAXS

-Basic data processing including size (Rg, Dmax), molecular weight, the P(r) function, and real space reconstructions

-Overview of ensemble and atomistic modeling

-Evaluating data quality and hands-on tutorials with data processing software

-What you need to know for publication

Kindly be aware that the provided schedule is provisional and may be subject to adjustments. Additionally, lunch is included as part of the registration fee for this workshop.

FULL SCHEDULE

WK3: Hands-On CryoEM Sample Preparation & Data Collection Workshop Using CryoEM Merit Badges

8:30am - 4:30pm Sunday, 7th July, 2024
Conifer Ballroom
Craig Yoshioka, Ed Eng

Cryo-electron microscopy (cryoEM) is a technology that enables biomedical researchers to determine high-resolution, three-dimensional structures of macromolecular complexes or cells. New cryoEM instrumentation is being installed in research institutions and there is a growing need to learn and share the best practices available in the field. This workshop, which will be held on Sunday, July 7, 2024, will focus on cryoEM educational resources available to researchers and to provide hands-on training with cryoEM instrumentation.

The NIH sponsored Transformative High-Resolution CryoEM Program offers a comprehensive cryoEM curriculum that familiarizes new users with cryoEM equipment and workflows. Lectures and practicals will focus on how to use the national cryoEM service centers, media-rich curriculum to augment users' own hands-on training, and hands-on use of cryoEM instrumentation using cryoEM merit badges. CryoEM proficiency badges are awarded to users in three main skill areas (Sample preparation, Microscope operations and Data processing). Students of this workshop will get "hands-on" training in all aspects of the cryoEM workflow. In particular, students will be able to demo vitrification instrumentation for the "Sample preparation" practicals, the national service centers will provide remote control of cryo-transmission electron microscopes (TEM) for the "Microscope operations" practicals, and cryoEDU will demonstrate SPA processing for the "Data processing" practicals. This workshop will benefit those who want to use cryoEM instrumentation at national service centers, or who may be new to cryoEM workflows.

Kindly be aware that the provided schedule is provisional and may be subject to adjustments. Additionally, lunch is included as part of the registration fee for this workshop.

FULL SCHEDULE

WK5: Crystallographic & cryo-EM structure Solution with Phenix

8:30am - 4:55pm Sunday, 7th July, 2024
Evergreen E
Dorothee Liebschner

The workshop is on structure determination of biological macromolecules with the software package Phenix. The lectures and tutorials will cover key stages of structure solution: from obtaining initial atomic models given experimental data (diffraction intensities or a 3D reconstruction) to final complete, refined and validated structures. Considering cryo-EM and crystallography, the instructors will compare and contrast tools and methods available in Phenix to perform these tasks. Particular focus is on Phenix tools designed for handling predicted models (e.g. AlphaFold) for X-ray crystallography and cryo-EM. Attendees are encouraged to actively participate in the workshop by asking questions about the presentations and by following tutorial exercises. The presentations introduce the Phenix system and the core algorithms that it uses; the presentations are followed by hands-on tutorials. The workshop will conclude with a general discussion.

Kindly be aware that the provided schedule is provisional and may be subject to adjustments. Additionally, lunch is not included as part of the registration fee for this workshop.

FULL SCHEDULE

WK1: Advanced Structure Refinement with Olex2 & NoSpherA2

9:00am - 5:15pm Sunday, 7th July, 2024
Evergreen C
Florian Kleemiss, Michael Bodensteiner, Oleg V. Dolomanov, Ilia A Guzei

Olex2 is one of the most widely used software for processing single crystal diffraction data. Many features make the handling of very difficult structural features a snap, such as disorder treatment, introduction of constraints, and recently anharmonicity has also been included. One of the most revolutionary features is the introduction of non-spherical atoms in Olex2 – NoSpherA2.

This workshop aims to introduce the variety of features that Olex2 provides to establish a routine workflow for refining and handling structural problems at any level of difficulty. This includes but is not limited to, treatment of solvent molecules, disorder, fragment-based model building, and obtaining publishable files directly after refinement. After the completion of a structural determination, the capabilities and workflow of NoSpherA2 will be presented, which significantly improve the model quality and, in many cases, allow reliable refinement of hydrogen atom positions from X-ray data.

Kindly be aware that the provided schedule is provisional and may be subject to adjustments. Additionally, please note that lunch is not included as part of this workshop.

FULL SCHEDULE

WK4: Simple & Advanced Single Crystal X-Ray Structure Refinement Using ShelXle

9:00am - 4:00pm Sunday, 7th July, 2024
Evergreen F
Ashley Weiland, Michael Ruf, Christian Hübschle, Matthias Matthias

ShelXle [1] is a graphical user interface for SHELXL [2], currently worldwide the most widely used program for small-molecule structure refinement, downloaded more than 80,000 times since its first release in 2011. ShelXle is fully compatible with all features of SHELXL and is written entirely in C++ using the Qt5/Qt6 libraries. It is available at no cost for Windows, Linux and Mac-OS X and as source code.

ShelXle combines an editor with syntax highlighting for the SHELXL-associated .ins (input) and .res (output) files with an interactive graphical display for visualization of a three-dimensional structure including high resolution the electron density (Fo) and difference density (Fo-Fc) maps. Editor (res file) and the graphical interface open at the same time, with instant simultaneous updating when making changes in either text or graphical editor. Special features of ShelXle include intuitive atom (re-)naming, support of PART and RESI commands as well as suffixes during atom renaming, unique and unrivaled structure visualization and highlighting tools, a symmetry manager supporting both EQIV and CIF style codes, as well as novel and unique ways of displaying disorder around both general and special positions. The DSR [3, 4] plugin can be of great help for modeling of complicated disorder. An intuitive hydrogen placement tool, atom sorting features, automatic unit cell content updating and removal of unused structure factors, and iterative weighting scheme optimization, tools for neutron, micro-ED and synchrotron data refinement and the ability to directly add or link additional external programs round out the capabilities of ShelXle.

In the workshop, attendees will go through worked examples that focus on both simple as well as advanced single crystal structure refinement using ShelXle. Topics will include the use of symmetry tools and difference density maps, structure visualization tools and disorder refinement, both with and without use of the DSR plugin. Attendees will be introduced to an easy-to-use interface to SHELXL and have a chance to discuss specific SHELXL or ShelXle related questions and/or problems.

[1] C. B. Hübschle, G. M. Sheldrick and B. Dittrich, (2011) J. Appl. Cryst. 44, 1281-1284.
[2] G. M. Sheldrick, (2008). Acta Cryst. A64, 112-122.
[3] D. Kratzert, I. Krossing, (2018) J. Appl. Cryst. 51, 928-934.
[4] D. Kratzert, J. J. Holstein, I. Krossing, (2015) J. Appl. Cryst. 48, 933-938.

Kindly be aware that the provided schedule is provisional and may be subject to adjustments. Additionally, lunch is included as part of the registration fee for this workshop.

FULL SCHEDULE

New Attendee Welcome

5:30 - 6:30pm Sunday, 7th July, 2024
Cottonwood
Gerald Audette, Allen Oliver

Welcome to the ACA Annual Meeting! We are thrilled to have you join us and invite you to our special New Attendee Welcome session. This event is designed to help you get acquainted with the conference, meet fellow newcomers, and connect with seasoned members of our community. You'll learn about the exciting sessions, networking opportunities, and social events planned for the week. It's a perfect chance to ask questions, share your interests, and start building valuable connections. We look forward to seeing you there!

Welcome & Keynote

6:30 - 7:30pm Sunday, 7th July, 2024
Evergreen AB
Stacey Smith, Samantha Powell, Anna Gardberg, Sarah Bowman, Allen Oliver

Join us for the Welcome & Keynote session where attendees will be greeted with an inspiring atmosphere of camaraderie and scientific curiosity. The keynote address, to be delivered by Catherine Drennan, a distinguished figure in the field of chemistry and biochemistry, will set the tone for the conference by highlighting groundbreaking research and emerging trends in the field. Catherine's insights on the future of structural science are expected to captivate the audience, fostering a sense of excitement and anticipation for the days ahead.

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417 Shake, Rattle, & Roll: Capturing Snapshots of Proteins in Action

Cathy L Drennan

Howard Hughes Medical Institute, Cambridge, MA, USA

Opening Reception

7:30 - 10:30pm Sunday, 7th July, 2024
Rocky Mountain Event Center

You're invited to join us for the opening reception at the ACA Annual Meeting! Kick off the conference in style with an evening of vibrant conversations, delicious hors d'oeuvres, and refreshing beverages. This lively event is the perfect chance to reconnect with old colleagues, forge new connections, and dive into stimulating discussions about the latest advancements in structural science. You'll also have the opportunity to visit with our exhibitors, explore the latest products and innovations, and engage directly with industry experts. Whether you're a seasoned attendee or a newcomer, this reception promises to be an engaging and welcoming start to an exciting week. We look forward to seeing you there!

Registration Desk

7:00am - 5:00pm Monday, 8th July, 2024
Rocky Foyer - Pint Brothers BY

Speaker Ready Room

7:00am - 5:00pm Monday, 8th July, 2024
Spruce 2

For presenters, the ACA offers a dedicated space where you can review and rehearse your materials to ensure everything is in order before your presentation. We highly encourage presenters to utilize this resource to ensure their presentations are ready and polished.

Transactions Symposium: Structural Science: Sharing Excitement & Appreciation - Part 1

8:30 - 11:30am Monday, 8th July, 2024
Evergreen A
Brandon Mercado, Charles Bou-Nader, Christine Zardecki, Louise Dawe, Allen Oliver

A fundamental challenge for specialists in any field is communicating the importance and intricacies of their work to those outside of it. The 2024 Transactions Symposium is designed to address two pivotal themes concerning the promotion and understanding of structural science. First, pedagogical approaches of teaching structural science, emphasizing the methodologies that resonate most effectively with learners will be explored. Second, strategies to captivate the interest of non-specialists, including funding agencies and the general public, will be considered.

By reflecting on what makes experts passionate about their field and what they wish others understood about it, the symposium aims to drive actionable insights into bridging gaps and fostering a broader appreciation for structural science.

8:30 - 9:00am

10 Everything's a Sample: Characterizing Everyday Materials using X-ray Powder Diffraction

James Kaduk

North Central College, Naperville, IL, USA

9:00 - 9:30am

92 Speaking to everyone about Crystallography – The Bragg Your Pattern Project

Helen Maynard-Casely[1], Stuart Batten[2], Rosemary Young[3], Bryce Mullens[4], Bronte Johnstone[5], Emily Furlong[6]

[1]Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Kirrawee DC, NSW, Australia. [2]Department of Chemistry, Monash University, Melbourne, VIC, Australia. [3]Australian Synchrotron, ANSTO, Melbourne, VIC, Australia. [4]Department of Chemistry, Sydney University, Sydney, NSW, Australia. [5]Department of Biochemistry and Pharmacology, The University of Melbourne, Melbourne, VIC, Australia. [6]Research School of Biology, Australian National University, Canberra, ACT, Australia

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9:30 - 10:00am

14 Bridging Concepts and Practice: Making Small-Molecule Crystallography Accessible to Chemistry Undergraduates and Secondary School Students

Shao-Liang Zheng

Harvard University, Cambridge, MA, USA

10:30 - 11:00am

194 Approaches to structural chemistry education for a broad audience at the Cambridge Crystallographic Data Centre

Yinka Olatunji-Ojo[1], Ilaria Gimondi[2], Andrew Peel[2], Suzanna Ward[2]

[1]The Cambridge Crystallographic Data Centre, Oakland, CA, USA. [2]The Cambridge Crystallographic Data Centre, Cambridge, Cambridgeshire, United Kingdom

11:00 - 11:30am

38 A periodic-like table of space groups

Bart Kahr

New York University, NYC, NY, USA

1.1.1 Advances in In situ cryo-electron tomography

8:30 - 11:30am Monday, 8th July, 2024
Evergreen B
Shyamal Mosaloganti, Vignesh Kasinath

This session will feature talks consisting both of biological and technological advances in macromolecular structure determination in the cellular context.

8:30 - 8:45am

218 Square beams for optimal tiling in TEM

Eugene Chua[1], Lambertus Alink[1], Mykhailo Kopylov[1], Jake Johnston[1], Fabian Eisenstein[2], Alex de Marco[1]

[1]New York Structural Biology Center, New York, NY, USA. [2]University of Tokyo, Tokyo, Tokyo, Japan

8:45 - 9:05am

142 Mechanisms of promoter nucleosome targeting and H2A.Z histone exchange by the SWR1 chromatin remodeler

Robert Louder

Johns Hopkins University, Baltimore, MD, USA

9:05 - 9:25am

178 A Multi-Modal and Generalizable Nanogold Tag for Cryo-Electron Tomography in Intact Cells

Lindsey Young[1], Alice Sherrard[2], Farhaz Shaikh[1], Huabin Zhou[3], Joshua Hutchings[1], Michael Rosen[3,4], Antonio Giraldez[2], Elizabeth Villa[1,5]

[1]UC San Diego, San Diego, CA, USA. [2]Yale University, New Haven, CT, USA. [3]UT Southwestern, Dallas, TX, USA. [4]HHMI, Dallas, TX, USA. [5]HHMI, La Jolla, CA, USA

9:25 - 9:45am

288 In-Situ Structural Studies of Eosinophil Granules

Jie E. Yang[1,2,3], Joshua Mitchell[4], Craig Bingman[5], Deane Mosher[4], Elizabeth Wright[1,2,3,6,7]

[1]Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [2]Cryo-Electron Microscopy Research Center, Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [3]Midwest Center for Cryo-Electron Tomography, Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [4]Departments of Biomolecular Chemistry and Medicine, University of Wisconsin, Madison, WI, USA. [5]Collaborative Crystallography Core, University of Wisconsin, Madison, WI, USA. [6]Morgridge Institute for Research, Madison, WI, USA. [7]DOE Great Lakes Bioenergy Research Center, University of Wisconsin, Madison, WI, USA

9:45 - 10:00am

323 Structural basis for inactivation of PRC2 by RNA

Jiarui Song[1,2], Vignesh Kasinath[1], Tom Cech[1,2]

[1]University of Colorado Boulder, Boulder, CO, USA. [2]Howard Hughes Medical Institute, Chevy Chase, MD, USA

10:30 - 11:00am

166 Resolving structurally heterogeneous ribosomes in situ with tomoDRGN

Joseph Davis, Barrett Powell

Massachusetts Institute of Technology, Cambridge, MA, USA

11:00 - 11:30am

368 Elucidating Tau Fibril Formation using Correlative Cryo-CLEM in situ

Sarah Shahmoradian

University of Texas Southwestern Medical Center, Dallas, TX, USA

1.1.2 Provenance, Workflow & Responsibility for X-Rays, Neutrons and Electrons – Part 1

8:30 - 11:30am Monday, 8th July, 2024
Evergreen C
Nicholas Sauter, Brent Nannenga

Could you prove your work is valid several years later? Could you recreate the figures? Is it possible to archive the raw data, along with enough description (metadata) so the whole calculation can be reproduced? What if the data are complex and include complementary information like spectroscopy? Our morning session will focus on the resources available for data storage and validation of results, while the afternoon will seek to present detailed experiences. Does science improve if every last bit is shared?

8:30 - 9:00am

65 Toward the Open Science model: publish your raw diffraction data.

Loes Kroon-Batenburg

Utrecht University, Utrecht, Utrecht, Netherlands

9:00 - 10:00am

7 Protein Data Bank: From Two Epidemics to the Global Pandemic to mRNA Vaccines and Paxlovid

Stephen Burley

RCSB Protein Data Bank, Piscataway, NJ, USA. Rutgers, The State University of New Jersey, Piscataway, NJ, USA. Rutgers Cancer Institute of New Jersey, New Brunswick, NJ, USA. UCSD, La Jolla, CA, USA

10:30 - 11:00am

94 Defining Grading Tools for Complex Small Molecules to Enable Assessment of Quality and Appropriate Reuse of Data

Aaron Horner

University of Southampton, Southampton, Hampshire, United Kingdom

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11:00 - 11:30am

239 Practicing FAIR research with SBGrid

Piotr Sliz

Harvard University, Boston, MA, USA. Boston Children's Hospital, Boston, MA, USA

1.1.3 Utilizing In Situ & Operando Techniques To Elucidate Complex Systems

8:30 - 11:30am Monday, 8th July, 2024
Evergreen D
Ashfia Huq, Saul Lapidus

The development of increasingly complicated materials and devices has led to a need of an understanding of the behavior of these system in the conditions that they will operate under. As such research into these has required the development of in situ/operando diffraction techniques to monitor and track changes in crystalline structure, amorphous behavior, and morphology. These conditions can vary from variable temperature, electrochemical cycling, gas flow, catalysis, and many others, and may combine these environments in different combinations. This session is aimed at providing a forum for presentation of advances in combing different in situ environments along with different methodologies of structural characterization (from diffraction to spectroscopy to microscopy) over a wide range of length scales (short range amorphous to crystalline to particle morphology). Submissions are welcome from various disciplines and fields, as these approaches may be wide-ranging in their application.

8:30 - 9:00am

203 Developing operando neutron total scattering for battery research

Jue Liu, zhijia Du, Michelle Everett

Oak Ridge National Lab, Oak Ridge, TN, USA

9:00 - 9:30am

110 Characterization of NMC cathodes and batteries via *operando* diffraction studies

Nathan Henderson

Bruker, Madison, Wisconsin, USA

9:30 - 10:00am

307 Exploration of Solid-State Reaction Kinetics: An *in-situ* Challenge

Mario Bieringer, Jenny Thoroski

University of Manitoba, Winnipeg, MB, Canada

10:30 - 11:00am

291 Using in situ X-ray diffraction to understand metathesis reactions towards ternary nitrides

Christopher Rom, Andriy Zakutayev

National Renewable Energy Laboratory, Golden, CO, USA

11:00 - 11:30am

173 Integrating Semi-Supervised Learning and Transformer Neural Networks for Lesion Classification in Alzheimer's Disease Pathology

Abdullah Al Bashit, Prakash Nepal, Lee Makowski

Northeastern University, Boston, 02155, MA, USA

1.1.4 Structure Visualization

8:30 - 11:30am Monday, 8th July, 2024
Evergreen EF
Helen Berman, Nichole Valdez

Advancements in visualization technology have created new ways for scientists to present dynamic processes and structural data in engaging and helpful formats. Visualization techniques are widely applicable to rendering molecular interactions, animating chemical reactions, visualizing small molecule and protein structures, aiding in structure-based drug design, and illustrating crystallography principles. This session focuses on communicating science through visualization using the latest developments in 2D and 3D methods. Techniques of interest include, but are not limited to, animation and rendering techniques, lighting and coloring effects, computer-aided design, VR, AR, and 3D printing.

8:30 - 9:00am

56 Challenges and Approaches in Visualizing 3D Protein Structures in Molecular Animations for All Audiences

Maria Voigt

RCSB Protein Data Bank, Piscataway, NJ, USA

9:00 - 9:30am

140 Quantitative mapping and visualizing of insulin hormone maturation

Kate White, Wen Lin, Aneesh Deshmukh, Kevin Chang, Ashley Archambeau, Nick Pudjarminta, Bryan Zhang

University of Southern California, Los Angeles, CA, USA

9:30 - 10:00am

262 Molecular Structure Visualization – I didn’t know Mercury could do that either!

Laura Friggeri[1], Jeff Lengyel[1], Suzanna Ward[2], Andrew Peel[2], Andrew Maloney[2]

[1]CCDC Inc, Boston, MA, USA. [2]CCDC, Cambridge, Cambridgeshire, United Kingdom

10:30 - 11:00am

421 Crystal Vision: A Virtual Reality Game for Learning Materials Crystallography

Nanzeeba Tabassum, Eric Shaffer, Nishant Garg

University of Illinois at Urbana-Champaign, Urbana, IL, USA

11:00 - 11:30am

331 Visualization of Topological Lattice Similarities

Charlene Tsay, Kevin Gagnon, Satish Kumar Iyemperumal

Vertex Pharmaceuticals, Boston, MA, USA

1.1.5 SAS In Biotherapeutics & Drug Development: SAXS/SANS/Hybrid Methods

8:30 - 11:30am Monday, 8th July, 2024
Conifer Ballroom
Kushol Gupta, Suzette Pabit

Characterization, validation, and optimization of emerging biologics, including therapeutic antibodies, viral vectors, and mRNA LNPs, requires comprehensive approaches to solution structure and dynamics. Small angle X-ray and Neutron Scattering (SAXS/SANS) provides information that is highly complementary to other well-established structural approaches, including electron microscopy, light scattering, analytical ultracentrifugation, and molecular dynamics. This session invites speakers who will showcase problems that employ multifaceted approaches to determine the properties of emerging biologics.

8:30 - 9:00am

297 Insights into mRNA lipid nanoparticle polydispersity and shape using quantitative solution biophysics

Marshall Padilla[1], Sarah Shepherd[1], Andrew Hanna[1], Martin Kurnik[2], Xujun Zhang[2], Michelle Chen[2], Alvin Mukalel[1], Hannah Yamagata[1], Adele Ricciardi[1], Ryann Joseph[1], Kaitlin Mrksich[1], Zain Siddiqui[1], David Issadore[1], Kushol Gupta[1], Michael Mitchell[1]

[1]University of Pennsylvania, Philadelphia, PA, USA. [2]Wyatt Technology, LLC, Goleta, CA, USA

9:00 - 9:30am

269 Structural characterization of nucleic acid-loaded lipid nanoparticles leveraging a high-throughput small angle X-ray scattering platform

Lee Joon Kim[1], Greg Hura[1,2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [2]University of California Santa Cruz, Santa Cruz, CA, USA

9:30 - 10:00am

342 Refining RNA Structures for Rational Drug Design: Atomistic structure of the SARS-CoV-2 pseudoknot in solution from SAXS-driven molecular dynamics

Josue San Emeterio

Xenocs, Inc, MA, USA

10:30 - 11:00am

200 Leveraging SAXS for Biologics Formulation Development in the Pharmaceutical Industry

Rahul Upadhya, Tyler Yarger, Marco Blanco, Jameson Bothe, Suzette Pabit, Hanmi Xi

Merck & Co., Inc., Rahway, NJ, USA

11:00 - 11:30am

29 High-Resolution Structure Determination of Protein-Ligand Complexes with Solution Scattering

Thomas Grant, Sarah Chamberlain, Jitendra Singh, Patrick Oduro

University at Buffalo, Buffalo, New York, USA

Exhibit Hall

10:00am - 12:00pm Monday, 8th July, 2024

Three Minute Thesis

11:45am - 12:45pm Monday, 8th July, 2024
Evergreen A
Alex Erickson, Kenny Childers

In this session, students and postdocs present their research in short, 3-minute presentations. Presenters will prepare a single slide with no animations and discuss their work in a relaxed setting while providing young scientists an opportunity to summarize their results for ACA members across all disciplines. Presenters are strongly encouraged to make their presentation approachable for all scientists outside of their field. This session invites submissions from all structural scientists.

78 Determining the Mechanism of DJ-1 Using Mix-and-Inject Synchrotron Serial Crystallography

Cole Dolamore[1], Kara Zielinski[2], Kevin Dalton[3], Stephen Meisburger[4], John Termini[5], Nathan Smith[1], Robert Henning[6], Vukica Srajer[6], Doeke Hekstra[3], Lois Pollack[2], Mark Wilson[1]

[1]University of Nebraska - Lincoln, Lincoln, NE, USA. [2]Cornell University, Ithaca, NY, USA. [3]Harvard University, Cambridge, MA, USA. [4]Cornell High Energy Synchrotron Source, Ithaca, NY, USA. [5]Beckman Research Institute, City of Hope, CA, USA. [6]Argonne National Laboratory (BioCARS), Lemont, IL, USA

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152 TraG-edy to Triumph: How Challenges in Crystallisation Efforts of TraG Led to Success

Nicholas Bragagnolo, Gerald Audette

York University, Toronto, Ontario, Canada

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400 SUBSTRATE BINDING FOR KETOHEXOKINASE-A REVEALS COOPERATIVITY IN THE INDUCED-FIT MECHANISM

SO YOUNG BAE, Karen N. Allen, Dean R. Tolan

Boston University, Boston, MA, USA

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343 Cryo-EM structural analysis of wild-type and ALS-related mutant SOD1 amyloid filaments

Yeongjin Baek, Hyunmin Kim, Soung-Hun Roh, Nam-Chul Ha

Seoul National University, Seoul, Seoul, Korea, Republic of

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341 Crystallization and structural investigation of HIV-1 Rev Response Element (RRE)

Hasan Al Banna, Deepak Koirala

University of Maryland, Baltimore County, Baltimore, MD, USA

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296 Simple techniques to improve particle distribution and data quality for dynamic protein-nucleic acid complexes

Chhandosee Ganguly[1], Lindsie Martin[1], Nathan D Burrows[2], Christina Zimanyi[3], Aaron Owji[3], Leonard M. Thomas[1], Rakhi Rajan[1]

[1]University of Oklahoma, Norman, Oklahoma, USA. [2]Stanford-SLAC Cryo-EM Center, Division of Cryo-EM and Bioimaging, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, California, USA. [3]National Center for CryoEM Access and Training, Simons Electron Microscopy Center, New York Structural Biology Center, New York, New York, USA

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365 Unveiling the Dynamic World of STEP: Structural Analysis in Response to Temperature, Pressure, Ligand Binding, and Dehydration.

Liliana Guerrero

City University of New York, New York, NY, USA. Advance Science Research Center, New York, NY, USA

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111 What is the best target protein density for TELSAM fusion crystallization

Prasadika Samarawickrama Hetti Arachchige, James Moody

Brigham Young University, Provo, Utah, USA

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156 Unveiling the Molecular Interplay of VPS34 Inhibition by Novel Drug Targets: A Promising Approach for Tailored Cancer Therapeutics

Wisdom Abiodun, James Moody

Brigham Young University, Provo, Utah, USA

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173 Integrating Semi-Supervised Learning and Transformer Neural Networks for Lesion Classification in Alzheimer's Disease Pathology

Abdullah Al Bashit, Prakash Nepal, Lee Makowski

Northeastern University, Boston, 02155, MA, USA

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406 Towards the spatial resolution of photosystem II charge states from XFEL diffraction data

Daniel Tchon[1], Johannes Blaschke[2], Vidya Ganapati[1], Daniel Paley[1], Billy Poon[1], Felix Wittwer[2], Iris Young[1], Aaron Brewster[1], Junko Yano[1], Jan Kern[1], Vittal Yachandra[1], Nicholas Sauter[1]

[1]Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging, Berkeley, CA, USA. [2]Lawrence Berkeley National Laboratory, National Energy Research Scientific Center, Berkeley, CA, USA

312 Crystallizing Student-Interest in Crystallography

Susanna Huang[1,2,3], Selina Huang[2,3]

[1]Georgia Institute of Technology, Atlanta, GA, USA. [2]SeNA Research Institute, Atlanta, GA, USA. [3]STARS crystallography research, Atlanta, GA, USA

Transactions Symposium: Structural Science: Sharing Excitement & Appreciation - Part 2

2:00 - 5:00pm Monday, 8th July, 2024
Evergreen A
Brandon Mercado, Charles Bou-Nader, Louise Dawe, Allen Oliver, Christine Zardecki

A fundamental challenge for specialists in any field is communicating the importance and intricacies of their work to those outside of it. The 2024 Transactions Symposium is designed to address two pivotal themes concerning the promotion and understanding of structural science. First, pedagogical approaches of teaching structural science, emphasizing the methodologies that resonate most effectively with learners will be explored. Second, strategies to captivate the interest of non-specialists, including funding agencies and the general public, will be considered. By reflecting on what makes experts passionate about their field and what they wish others understood about it, the symposium aims to drive actionable insights into bridging gaps and fostering a broader appreciation for structural science.

2:00 - 2:10pm

106 Sharing our Excitement for Structural Science Through our Trainees

Gerald Audette

York University, Toronto, ON, Canada

2:10 - 2:55pm

299 Communicating Scientific Concepts Through Art

Beata Mierzwa

University of California San Diego, La Jolla, CA, USA

3:30 - 4:00pm

13 Insights from 25 Years of the Molecule of the Month

David Goodsell

The Scripps Research Institute, La Jolla, CA, USA

4:00 - 4:30pm

249 Centering students and collaboration in science: humanizing the development of unnatural amino acids as tools to study protein structure

Christine Phillips-Piro

Franklin & Marshall College, Lancaster, PA, USA

4:30 - 5:00pm

192 From Angstrom to meters: How access to basic science can influence public trust and health equity

Jamaine Davis

Meharry Medical College, Nashville, TN, USA

1.2.1 New Sample Preparation Technology For Cryo-EM & Cryo-ET

2:00 - 5:00pm Monday, 8th July, 2024
Evergreen B
David Taylor, Ed Eng

Developments in cryo-EM and cryo-ET imaging technology have revolutionized our ability to see the atomic structure of proteins and biological macromolecules in the cellular environment. However, the success of many research projects remains limited by issues of sample yield, stability, and orientation bias. In this session, we explore and discuss new developments in sample preparation technologies that address current challenges and open doors to exciting areas of biology.

2:00 - 2:30pm

49 Open-Source Light-Coupled Specimen Preparation for Cryo-EM and Cryo-ET

Edward Twomey

Johns Hopkins University, Baltimore, MD, USA

2:30 - 3:00pm

217 A Plug and Play Flash and Freeze System for cryoTREM: Design, Build, Testing and Initial Implementation

Biddut Bhattacharjee[1], Md Mahfuzur Rahman[2], Ryan Hibbs[3], Michael Stowell[1]

[1]CU Boulder, Boulder, CO, USA. [2]UT Southwestern, Dallas, TX, USA. [3]UCSD, San Diego, CA, USA

3:30 - 4:00pm

69 Lysate-to-grid: Rapid Isolation of Native Complexes from Cell Lysate for Cryo-EM Imaging

Ian Cooney, Deirdre Mack, Aaron Ferrell, Michael Stewart, Shuxin Wang, Helen Donelick, Daniela Tamayo-Jaramillo, Dakota Greer, Danyang Zhu, Wenyan Li, Peter Shen

University of Utah, Salt Lake City, UT, USA

4:00 - 4:15pm

163 Cryo-EM Protein Structure Without Purification

Samantha Powell[1], James Evans[1,2]

[1]Pacific Northwest National Laboratory, Richland, WA, USA. [2]Washington State University, Pullman, WA, USA

4:15 - 4:30pm

135 Advancing Cryo-ET Sample Preparation: Integrated FLM for Cryo-FIB for targeted milling of challenging samples.

Samuel Zachej[1], Wessel Teunisse[2], Marit Smeets[2], Jakub Javůrek[1], Dominik Pinkas[3], Vlada Filimonenko[3]

[1]TESCAN GROUP, Brno, South Moravian Region, Czech Republic. [2]Delmic B.V., Delft, Zuid-Holland, Netherlands. [3]Institute of Molecular Genetics of the Czech Academy of Sciences, Prague, Prague, Czech Republic

4:30 - 5:00pm

59 Time-resolved cryogenic electron tomography using mix-and-inject microfluidic devices

Peter Dahlberg[1], Joey Yoniles[1], Jacob Summers[1], Kara Zielinski[2], Cali Antolini[1], Mayura Panjalingam[3], Stella Lisova[1], Frank Moss[1], Maximus Perna[1], Christopher Kupitz[1], Mark Hunter[1], Lois Pollack[2], Soichi Wakatsuki[1]

[1]SLAC, Menlo Park, California, USA. [2]Cornell University, Ithica, NY, USA. [3]New York University, New York, New York, USA

1.2.2 Provenance, Workflow & Responsibility for X-Rays, Neutrons and Electrons – Part 2

2:00 - 5:00pm Monday, 8th July, 2024
Evergreen C
Nicholas Sauter, Brent Nannenga

2:00 - 2:30pm

281 Getting started with the Gold Standard: NeXus in crystallography

Aaron Brewster[1], Herbert Bernstein[2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [2]Fresh Pond Research Institute, New York, NY, USA

2:30 - 3:00pm

298 MicroED data: from microscope to archive

Johan Hattne[1,2], Michael Martynowycz[2], Max Clabbers[1,2], William Nicolas[1,2], Tamir Gonen[1,2]

[1]Howard Hughes Medical Institute, Los Angeles, CA, USA. [2]University of California, Los Angeles, Los Angeles, CA, USA

3:30 - 4:00pm

324 Data retention for high-throughout XFEL chemical crystallography

Daniel Paley[1], Elyse Schriber[2], Daniel Rosenberg[2], Daniel Tchoń[1], David Mittan-Moreau[1], J. Nathan Hohman[3], Aaron Brewster[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [2]SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [3]University of Connecticut, Storrs, CT, USA

4:00 - 4:30pm

32 Sixth Decade of Protein Data Bank Operations: Transition to Extended PDB IDs and PDBx/mmCIF Format

Sutapa Ghosh[1], Zukang Feng[1], Yuhe Liang[1], Ezra Peisach[1], Irina Persikova[1], Jasmine Young[1], wwPDB Team[1,2,3,4,5,6], Stephen Burley[1,7]

[1]RCSB Protein Data Bank, Rutgers, The State University of New Jersey, Piscataway, NJ, USA. [2]PDBe, EMBL-European Bioinformatics Institute, Hinxton, Cambridge, United Kingdom. [3]PDBj, Institute for Protein Research, Osaka University, Osaka, Osaka, Japan. [4]EMDB, EMBL-European Bioinformatics Institute, Hinxton, Cambridge, United Kingdom. [5]BMRB, UConn Health, Farmington, CT, USA. [6]PDBc, ShanghaiTech University and National Facility for Protein Science in Shanghai, Shanghai, Shanghai, China. [7]RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, La Jolla, CA, USA

4:30 - 5:00pm

225 Multiplex and complementary datasets are vital to dynamic structural biology results

Allen Orville[1], Pierre Aller[2], Anastasya Shilova[1]

[1]Diamond Light Source, Didcot, Oxfordshire, United Kingdom. [2]Diamond Light Source, Ddicot, Oxfordshire, United Kingdom

1.2.3 Extreme Biophysical & Biochemical Environments

2:00 - 5:00pm Monday, 8th July, 2024
Evergreen D
Susana Teixeira, Silvia Russi, Sai Venkatesh Pingali

Complex environments enable the study of biomacromolecules and biomaterials in extreme natural or application-based conditions like for biomaterial processing, bioenergy, organisms in deep sea, space exploration. This session will cover scientific talks for the biological community from light and neutron user facilities requiring a range of complex environments that facilitate changes to pH, ionic strength, solvents, pressure, temperature including in-situ and in-vivo measurements of biomolecules – from relatively simple formulations to whole cells.

2:00 - 2:20pm

294 Sample Environments for Extreme Biology of Small-Angle Neutron Scattering at Oak Ridge National Laboratory

Sai Venkatesh Pingali

Oak Ridge National Laboratory, Oak Ridge, TN, USA

2:20 - 2:40pm

275 *In-situ* Neutron Scattering of Poplar Woodchip upon Reductive Fractionation

Manjula Senanayake

Washington University in St. Louis, St Louis, MO, USA

2:40 - 3:00pm

190 X-Bio: eXtreme structural biology and biophysics at CHESS

Steve Meisburger, Richard Gillilan, Qingqiu Huang, Zhongwu Wang, Jeney Wierman

Cornell High Energy Synchrotron Source, Ithaca, NY, USA

3:30 - 4:00pm

278 High-pressure room-temperature crystallography reveals catalytic lid dynamics even in the absence of ligands

John Indergaard[1], Matthew McLeod[1], Robert Thorne[1], Todd Holyoak[2]

[1]Cornell University, Ithaca, NY, USA. [2]University of Waterloo, Waterloo, Ontario, USA

4:00 - 4:30pm

73 Pushed to extremes: distinct effects of high temperature vs. pressure on the structure of a phosphatase enzyme

Daniel Keedy

CUNY Advanced Science Research Center, New York, NY, USA

4:30 - 5:00pm

263 Optochemistry and Transcription at 160 Kelvin

Guillermo Calero[1], Guowu Lin[1], Ulises Santiago[1], Sandra Vergara[1], Silvia Russi[2], Aina Cohen[2]

[1]University of Pittsburgh, Pittsburgh, PA, USA. [2]SSRL, Menlo Park, CA, USA

1.2.4 Home-Built Software & Hardware

2:00 - 5:00pm Monday, 8th July, 2024
Evergreen EF
Larry Falvello, Victor Young

The changing role of home-built software and hardware is the theme of this half-day session. Purpose-built in-house software for crystallography has spanned the entire range of uses, from specific tasks such as data format-changing to more global data- and structure-analysis packages. Crystallographic software has a singular characteristic in that a large fraction of published crystallographic results are obtained using software that originated in active crystallography laboratories. Less famous are applications prepared locally to improve work flow and data security. Similarly, hardware ranging from simple gadgets for crystal handling and mounting all the way to diffractometers for use with unique radiation sources have been custom-made for crystallographic applications. The conditioning of sample environments, including the creation of extreme conditions, has been an area of active development, as has the development of systems for diffraction under in situ conditions. This session will welcome contributions from all who create and/or adapt software or hardware for crystallographic use. Innovative applications for any diffraction experiment in the home laboratory, at a synchrotron or a neutron source may be presented. As in the previous editions of this topic, contributions of a historical nature will be welcome.

2:00 - 2:20pm

57 Custom systems powered by MetalJet bringing synchrotron applications to the lab

Julius Hållstedt[1], Rob Drake[2]

[1]Excillum, Kista, Sweden, Sweden. [2]Proto XRD, LaSalle, Ontario, Canada

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2:20 - 2:40pm

150 Minor Homemade Tools For Use With PXRD

Matthew Brown, Kyle Lessoway, Christopher Seib

University of British Columbia, Kelowna, BC, Canada

2:40 - 3:00pm

193 Powder Pattern Denoising Using Haar/Poisson Algorithm: Efficient Implementation and Performance

Richard McClurg

Curia, West Lafayette, IN, USA

3:30 - 4:00pm

285 Direction cosines, the orientation matrix and more: Past and present

Larry Falvello

University of Zaragoza - CSIC, Zaragoza, Zaragoza, Spain

4:00 - 4:30pm

309 VOICE COMPUTING IN BIOLOGICAL CRYSTALLOGRAPHY

Blaine Mooers

University of Oklahoma Health Sciences, Oklahoma City, OK, USA

4:30 - 5:00pm

311 Using the MATCH procedure in Oxford University's *Crystals for Windows* software to search for phase transitions in twins

Victor Young[1], Bruce Foxman[2]

[1]University of Minnesota, Minneapolis, MN, USA. [2]Brandeis University, Waltham, MA, USA

1.2.5 Hot Structures

2:00 - 5:00pm Monday, 8th July, 2024
Conifer Ballroom
Aaron Robart, Evan Cramer

The Hot Structures session will feature talks primarily selected from submitted abstracts describing the newest results from structural studies of biologically important macromolecules. Submissions are welcome that describe high-impact structures which provide new insights into biological phenomena, structure-function relationships, and methods development. Studies may include the use of X-ray crystallography, XFEL, Cryo-EM, Small Angle X-ray Scattering, or hybrid methods including those that incorporate predictive / computational modeling.

2:00 - 2:20pm

131 Revisiting nucleotide-dependent allostery in aspartate transcarbamoylase

Michael Patterson, Robert Miller, Neti Bhatt, Xiaokun Pei, Nozomi Ando

Cornell University, Ithaca, NY, USA

2:20 - 2:40pm

256 The C5α-Methyl Substituted Carbapenem NA-1-157 Inhibits the Class A Carbapenemase GES-5

Clyde Smith[1], Nichole Stewart[2], Marta Toth[2], John Buynak[3], Sergei Vakulenko[2]

[1]SSRL, Menlo Park, CA, USA. [2]University of Notre Dame, Notre Dame, IN, USA. [3]Southern Methodist University, Dallas, TX, USA

2:40 - 3:00pm

169 Molecular basis of uphill energy transfer for photosynthesis in the Antarctic alga

Makiko Kosugi[1], Masato Kawasaki[2], Yutaka Shibata[3], Toshiya Senda[2]

[1]National Institute for Basic Biology, Okazaki, Aichi, Japan. [2]High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan. [3]Tohoku University, Senda, Miyagi, Japan

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3:30 - 3:55pm

189 Capturing oligomeric states of Lon protease involved in its regulation using CryoEM

Ishan Rathore[1], Alla Gustchina[1], Di Zhang[1], Tatyana Rotanova[2], Alexander Wlodawer[1]

[1]National Cancer Institute, National Institute of Health, Frederick, Maryland, USA. [2]Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Moscow, Moscow, Russian Federation

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3:55 - 4:15pm

238 Structural Characterization of the *Clostridioides difficile* Transferase Reveals Intoxication Intermediates

Michael Sheedlo, Robin Mullard

University of Minnsota, Minneapolis, Mn, USA

4:15 - 4:35pm

250 RNA-based strategy of enteroviral genome replication

Naba Krishna Das, Jeff Vogt, Alisha Patel, Hasan Al Banna, Deepak Koirala

University of Maryland, Baltimore County, Baltimore, Maryland, USA

4:35 - 5:00pm

16 Regulation of the Essential Transmembrane AAA+ Protease FtsH by HflK/C Oligomeric Assembly

Alireza Ghanbarpour[1], Jia Jia Zhang[1], Bertina Telusma[1], Barrett Powell[1], Isabella Bolstad[1], Tania Baker[1], Sandro Keller[2], Robert T. Sauer[1], Joseph H. Davis[1]

[1]MIT, Cambridge, MA, USA. [2]UNIVERSITY OF GRAZ, Graz, Graz, Austria

Exhibit Hall

2:00 - 7:30pm Monday, 8th July, 2024

PS1: Poster Session #1

5:30 - 7:30pm Monday, 8th July, 2024
Atrium
Leighanne Gallington, Sara Andres

296 Simple techniques to improve particle distribution and data quality for dynamic protein-nucleic acid complexes

Chhandosee Ganguly[1], Lindsie Martin[1], Nathan D Burrows[2], Christina Zimanyi[3], Aaron Owji[3], Leonard M. Thomas[1], Rakhi Rajan[1]

[1]University of Oklahoma, Norman, Oklahoma, USA. [2]Stanford-SLAC Cryo-EM Center, Division of Cryo-EM and Bioimaging, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, California, USA. [3]National Center for CryoEM Access and Training, Simons Electron Microscopy Center, New York Structural Biology Center, New York, New York, USA

353 **Wide-angle scattering studies of nucleic acids**

Sarah Uttormark, Lois Pollack

Cornell University, Ithaca, New York, USA

382 **Understanding the Molecular Mechanism of Redondovirus Rep in Rolling Circle Replication of the Redondoviral Genome**

Saira Montermoso, Kushol Gupta, Frederic Bushman, Gregory Van Duyne

University of Pennsylvania, Philadelphia, PA, USA

398 **Structure and Functional Analysis of a Bacterial Gene-Regulatory RNA Switch that Binds the DNA Damage Product 8-Oxoguanine**

Coleman B. Goenner, Jermaine L. Jenkins, Joseph E. Wedekind

Dept. of Biochemistry & Biophysics and Center for RNA Biology, University of Rochester School of Medicine & Dentistry, Rochester, New York, USA

399 **Allosteric and Cooperative Networks in a Homodimeric Epoxide Hydrolase**

Adam Simard[1], Kelli Hvorecny[1], Noor Taher[1], Akaash Mishra[1], Natalia Vasylieva[2], Christophe Morisseau[2], Dean Madden[1]

[1]Dartmouth College, Hanover, NH, USA. [2]University of California, Davis, Davis, CA, USA

412 **Characterization of the Eya and PP2A-B55α interaction**

Christopher Alderman[1], Ryan Anderson[1], Lingdi Zhang[1,2], Connor Hughes[1], Xueni Li[1], Chris Ebmeier[3], Marisa Wagley[1], Natalie Ahn[3], Heide Ford[1], Rui Zhao[1]

[1]CU, Aurora, CO, USA. [2]Arnatar Therapeutics, San Diego, CA, USA. [3]CU, Boulder, CO, USA

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76 High conservation doesn’t always translate: A comparison of ATAD2 and ATAD2B structure and function

Kiera Malone[1], Margaret Phillips[1], Ajit Singh[1], Isabelle Kressy[1], Brian Boyle[1], James Lignos[1], Jay Nix[2], Karen Glass[1]

[1]University of Vermont, Burlington, VT, USA. [2]Advanced Light Source, Berkeley, CA, USA

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354 Characterizing single-stranded RNA using SAXS and single-molecule FRET

Scout Fronhofer, Tong Wang, Lois Pollack

Cornell University, Ithaca, New York, USA

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365 Unveiling the Dynamic World of STEP: Structural Analysis in Response to Temperature, Pressure, Ligand Binding, and Dehydration.

Liliana Guerrero

City University of New York, New York, NY, USA. Advance Science Research Center, New York, NY, USA

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403 Characterization of reconstituted receptor-histidine kinase core signaling complexes

Yajie Xu, Brian Crane

Cornell University, Ithaca, NY, USA

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364 *Capturing multiple conformations of a glycyl radical enzyme utilizing new sample preparation methods for cryo-electron microscopy*

Christa Imrich, Lindsey Backman, Mary Andorfer, Catherine Drennan

Massachusetts Institute of Technology, Cambridge, MA, USA

383 Towards structural determination of fluoride export proteins

Chia-Yu Kang, Minjun An, Melanie Ohi, Randy Stockbridge

University of Michigan, Ann Arbor, MI, USA

333 Utilizing SacB Negative Selection in *E. coli* to Evaluate 10-23 DNAzyme Activity in Cellular Conditions

Evan Cramer, Aaron Robart

West Virginia University, Morgantown, WV, USA

369 Structural and functional analysis of the *Legionella pneumophila Dot/Icm* Type IV secretion system proteins Dis2 and Dis3

Jacquelyn Roberts[1], Arwen Frick-Cheng[2], Henry Styron[2], Clarissa Durie[3], Louise Chang[2], Melanie Ohi[4]

[1]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI, USA. [2]Life Sciences Institute, University of Michigan, Ann Arbor, MI, USA. [3]Department of Biochemistry, University of Missouri, Columbia, MO, USA. [4]Department Molecular, Cellular, and Developmental Biology, University of Michigan, Ann Arbor, MI, USA

392 Uncovering LysRS Non-Canonical Functions: A Structural Exploration

Annalise Holland

Emory University, Atlanta, GA, USA

175 Structural Studies of an F-plasmid Protein TraW

Christina Rodriguez, Gerald Audette

York University, Toronto, ON, Canada

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349 Expression, Purification, and Biophysical Characterization of Monkeypox Virus Protein I1

Ziqi An, Rajan Lakhani, Robert Sharp, Kushol Gupta, Gregory D. Van Duyne

Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA

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400 SUBSTRATE BINDING FOR KETOHEXOKINASE-A REVEALS COOPERATIVITY IN THE INDUCED-FIT MECHANISM

SO YOUNG BAE, Karen N. Allen, Dean R. Tolan

Boston University, Boston, MA, USA

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367 Unveiling Graphene's Potential for Medical Devices: Synthesis & Characterization for Light-Based Applications

Salah OUDJERTLI

Research Center In Industrial Technologies. (CRTI) BP 64, Roade of Dely Brahim, Cheraga 16014 Algiers – Algeria, Algiers, Algeria, Algeria

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341 Crystallization and structural investigation of HIV-1 Rev Response Element (RRE)

Hasan Al Banna, Deepak Koirala

University of Maryland, Baltimore County, Baltimore, MD, USA

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376 Development of a Streamlined Cryo-EM Method to Solve Nucleic Acid Structures

Holly Shultz, Evan Cramer, Jasmine Harper, Sarah Starcovic, Aaron Robart

West Virginia University, Morgantown, WV, USA

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405 Understanding the Structure and Function of Alternative Splicing Factor PRPF39

Collette Wright, Shasha Shi, Francesca De Bortoli, Jenna Kotz, Xueni Li, Rui Zhao

University of Colorado Anschutz Medical Campus, Aurora, CO, USA

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47 Structural insights into RNA targeting with *de novo* small molecule

Ling Xu[1,2], Kevin Chung[1], Tianshuo Liu[1], Anna Marie Pyle[1,2]

[1]Yale University, New Haven, CT, USA. [2]HHMI, Chevy Chase, MD, USA

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396 Unraveling the mechanism of how small molecule modulates 5’ splice site recognition

Shasha Shi[1], Xueni Li[1], Zhiling Kuang[1], Bryan M Dunyak[2], Frederic Vaillancourt[2], Subbaiah Chalivendra[1], Rui Zhao[1]

[1]University of Colorado Denver Anschutz Medical Campus, Aurora, CO, USA. [2]Remix Therapeutics, Watertown, MA, USA

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287 Cryo-EM reveals the structural and functional role of prothrombin recognition by type-I anti-prothrombin antibody in Antiphospholipid Syndrome.

Suresh Kumar[1], Vittorio Pengo[2], Robert Flaumenhaft[3], Nicola Pozzi[4]

[1]Department of Biochemistry and Molecular Biology, Saint Louis University, Saint Louis, Missouri, USA. [2]Department of Cardiac-Thoracic-Vascular Sciences and Public Health, University of Padova,, Padova, Padua, Italy. [3]Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, Massachusetts, USA. [4]Department of Biochemistry and Molecular Biology, Saint Louis University, Saint Louis, MO, USA

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402 Cryo-EM Structural Characterization of the FeFe-Hydrogenase Maturase Complex

James Moody, Maria Jose Pedroza Romo, Joseph Gonzalez

Brigham Young University, Provo, Utah, USA

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395 Computational and structural study of ORF4 protein on human coronavirus 229E

Bhargy Sharma, Konstantin Pervushin

Nanyang Technological University, Singapore, Singapore, Singapore

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343 Cryo-EM structural analysis of wild-type and ALS-related mutant SOD1 amyloid filaments

Yeongjin Baek, Hyunmin Kim, Soung-Hun Roh, Nam-Chul Ha

Seoul National University, Seoul, Seoul, Korea, Republic of

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352 STRUCTURAL CHARACTERIZATION OF DIIRON-DEPENDENT PLASMANYLETHANOLAMINE DESATURASE (CarF)FROM *Myxococcus xanthus*

Jayoh Hernandez[1], Catherine Drennan[1], Naike Ye[1], Irene del Rey Navalón[2], Montserrat Elías Arnanz[2]

[1]Massachusetts Institute of Technology, Cambridge, Massachusetts, USA. [2]Universidad de Murcia-Campus de Espinardo, Murcia, Murcia, Spain

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371 Structural Elucidation of an RNA Triple Helix in Complex with a Small Molecule

Madeline M. Glennon[1], Krishna M. Shivakumar[1], Martina Zafferani[2], Conner J. Langeberg[3], Jeffrey S. Kieft[4], Amanda E. Hargrove[2], Jessica A. Brown[1]

[1]Department of Chemistry and Biochemistry, University of Notre Dame, South Bend, IN, USA. [2]Department of Chemistry, Duke University, Durham, NC, USA. [3]Innovative Genomics Institute, University of California, Berkeley, CA, USA. [4]New York Structural Biology Center, New York, NY, USA

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184 Mechanistic Investigation of the Class III Ribonucleotide Reductase

Zhuangyu Zhao[1], Catherine Drennan[2,3]

[1]Department of Biology, Massachusetts Institute of Technology, Cambridge, MA, USA. [2]Departments of Biology and Chemistry, Massachusetts Institute of Technology, Cambridge, MA, USA. [3]Howard Hughes Medical Institute, Chevy Chase, MD, USA

388 Approaches to characterize *in situ* viral glycoprotein structure and function

Lily Taylor, Jose Rodriguez

UCLA, Los Angeles, CA, USA

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431 Inhibition of prolyl endopeptidase through a noncatalytic active site residue

Ian Fucci[1], Kalyani Thakur[2], Euna Yoo[2], Diana Monteiro[1]

[1]Center for Structural Biology, NCI, NIH, Frederick, Maryland, USA. [2]Chemical Biology Laboratory, NCI, NIH, Frederick, Maryland, USA

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435 Single-Crystal-to-Single-Crystal Post-Synthetic Modifications Monitored via SC-XRD

Anna Berseneva[1,2], Hans-Conrad zur Loye[1]

[1]University of South Carolina, Columbia, SC, USA. [2]NREL, Golden, CO, USA

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437 Photo-assisted electron transfer in Cu(II)-doped biological model crystals.Michael J. Colaneri[1] , Jacqueline Vitali[2] and Simon J. Teat[3][1]SUNY at Old Westbury, Old Westbury, NY, USA. [2]Cleveland State University, Cleveland, OH, USA. [3]Lawrence Berkeley National Lab, Berkeley, CA, USA.

Michael Colaneri[1], Jacqueline Vitali[2], Simon Teat[3]

[1]SUNY at Old Westbury, Old Westbury, NY, USA. [2]Cleveland State University, Cleveland, OH, USA. [3]Lawrence Berkeley National Lab, Berkeley, CA, USA

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410 Unveiling the Inherent Beauty of Crystallography to Undergraduate Students

Susanna Huang

Georgia Institute of Technology, Atlanta, GA, USA. STARS, Inc. (Nonprofit), Atlanta, GA, USA

YSIG Mixer

8:00 - 10:00pm Monday, 8th July, 2024
Niko Vlahakis

Location: [The Viewhouse (7101 South Clinton, Centennial CO 80112)]

TRANSPORTATION NOTE: If you are attending the YSIG mixer, we are pleased to offer a complimentary shuttle service. The shuttle will operate from 7:00 to 8:00 PM, with return trips starting at 9:30 PM. Priority boarding will be given to those with physical challenges, but everyone is welcome to use the service. The shuttle will leave from the hotels front entrance and run on a first-come, first-served basis. If you prefer not to take the shuttle, alternative transportation options include walking, taxi, or Uber. We look forward to seeing you at the mixer!

Please note that the YSIG Mixer is designed as a mixer and social gathering, and it is not intended to be a formal dinner. While light refreshments will be available, please plan your evening accordingly. We believe this will create a more relaxed atmosphere for everyone to engage in meaningful conversations and networking

Registration Desk

7:00am - 5:00pm Tuesday, 9th July, 2024
Rocky Foyer - Pint Brothers BY

Speaker Ready Room

7:00am - 5:00pm Tuesday, 9th July, 2024
Spruce 2

For presenters, the ACA offers a dedicated space where you can review and rehearse your materials to ensure everything is in order before your presentation. We highly encourage presenters to utilize this resource to ensure their presentations are ready and polished.

2.1.1 General Interest - Part 1

8:30 - 11:30am Tuesday, 9th July, 2024
Conifer Ballroom
Tim Stachowski, Tori Drago, Zhen Xu

General Interest sessions are the forum for topics of broad interest to the structural science or for presentations that do not fit the specific theme of other sessions. All presentations are selected from submitted abstracts.

8:30 - 8:55am

146 Where are the crystals? X-DES: Deep Eutectic Solvents based on Halogen Bonding

William Pennington, Madhushi Bandara, Andrew Peloquin, Colin McMillen

Clemson University, Clemson, SC, USA

8:55 - 9:15am

112 Exploring the Structural Behavior of Hydrophilic Diglycolamide Complexes with the Lanthanides and Actinides

Brian Rotermund[1,2], Joseph Sperling[1], Nicholas Beck[1], Gregory Horne[2], Thomas Albrecht-Schoenzart[1]

[1]Colorado School of Mines, Golden, CO, USA. [2]Idaho National Lab, Idaho Falls, ID, USA

9:15 - 9:35am

172 Inconsistencies in the Order of Space Groups: Why is $C222_1$ before $C222$?

Carolyn Pratt Brock[1], Mois I. Aroyo[2]

[1]University of Kentucky, Lexington, KY, USA. [2]University of the Basque Country EHU/UPV, Bilbao, Bizkaia, Spain

9:35 - 10:00am

183 Renaissance of Megaelectronvolt Electron Scattering

Xijie Wang

Univeristy of Dusburg-Essen, Duisburg, North Rhine-Westphalia, Germany. TU Dortmund University, Dortmund, North Rhine-Westphalia, Germany

10:30 - 10:50am

155 Direct detection in CdTe enables high efficiency for short- and dual-wavelength instruments

Pascal Hofer[1], Marcus Müller[2]

[1]DECTRIS USA Inc, Philadelphia, PA, USA. [2]DECTRIS Ltd, Baden-Daettwil, AG, Switzerland

10:50 - 11:10am

171 LRL_WEB, A Website for a More Thorough Exploration of Bravais Lattice Types of Your Unit Cells

Lawrence C Andrews[1], Herbert J Bernstein[2]

[1]Ronin Institute for Independent Scholarship, Kirkland, WA, USA. [2]Fresh Pond Research Institute, New York, NY, USA

11:10 - 11:30am

144 Coordination Transformations in Lanthanide Complexes Under Pressure

Nicholas Beck, Daniela Gomez Martinez, Thomas Albrecht-Schoenzart

Colorado School of Mines, Golden, CO, USA

2.1.2 Light Sources Through the Decades - Part 1

8:30 - 11:30am Tuesday, 9th July, 2024
Evergreen A
Marian Szebenyi, Brian Toby

8:30 - 9:00am

99 High resolution powder diffraction at the ESRF

Andy Fitch

ESRF, Grenoble, Isère, France

9:00 - 9:30am

240 The Early Days of Powder Diffraction at NSLS-I

David Cox

Brookhaven National Laboratory, South Setauket, NY, USA

9:30 - 10:00am

251 Anomalous dispersion - versatile and useful

Michael Bodensteiner[1], Florian Meurer[1,2,3], Christoph Hennig[2,3]

[1]University of Regensburg, Regensburg, Bavaria, Germany. [2]Rossendorf Beamline (BM20-CRG) ESRF, Grenoble, Isere, France. [3]Institute of Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Saxonia, Germany

10:30 - 10:50am

161 The PILATUS Story: The Rise of Hybrid Photon Counting Detectors for Efficient and Fast X-Ray Diffraction

Max Burian, Pascal Hofer, Tilman Donath, Sascha Grimm

DECTRIS Ltd, Baden, AG, Switzerland

10:50 - 11:10am

197 Building the Power of Modern Macromolecular Crystallography

Robert Sweet

National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA

11:10 - 11:30am

114 From X-ray Synchrotrons to Storage Rings – Revolutionizing Determination of Biological Structure

Keith Hodgson

Stanford University, Stanford, CA, USA

2.1.3 Structural Biology in Pharma/Biotech - Part 1

8:30 - 11:30am Tuesday, 9th July, 2024
Evergreen B
Chelsy Chesterman, Eddie Pryor

A full-day session dedicated to exploring various topics in Structural Biology in Pharma/Biotech. We invite submissions on any topic related to the industrial application of structural biology, including but not limited to: vaccines, CART-T, TPD/TPS glues, macrocyclic peptides, induced proximity, and FBDD. Additionally, we encourage presentations that utilize a variety of techniques such as x-ray, NMR, EM, in silico, and biophysics. Technology or methods development in these areas is also of interest. Accepted abstracts will be grouped and assigned to a specific session.

8:30 - 8:50am

149 Secretory biogenesis and design of a next-generation coronavirus genetic vaccine

Suruchi Singh[1], Meghan C. Burke-Harris[2], Yi Liu[2], Fiona L Kearns[3], Rui Yin[4], Toheeb Balogun[3], Benjamin Jennings[5], Brian Pierce[6,7,8], Balraj Doray[5], Rommie Amaro[3,9], Stephen E. Stein[2], S. Saif Hasan[1,8,10]

[1]Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, Baltimore, MD, USA. [2]Mass Spectrometry Data Center, Biomolecular Measurement Division, National Institute of Standards and Technology, Gaithersburg, MD, USA. [3]Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA, USA. [4]University of Maryland Institute for Bioscience and Biotechnology Research, Rockville, MD, USA. [5]Department of Internal Medicine, Hematology Division, Washington University School of Medicine, St. Louis, MO, USA. [6]University of Maryland Institute for Bioscience aBiotechnology, Rockville, MD, USA. [7]Department of Cell Biology and Molecular Genetics, University of Maryland, College Park, MD, USA. [8]University of Maryland Marlene and Stewart Greenebaum Cancer Center, University of Maryland Medical Center, Baltimore, MD, USA. [9]Glycobiology Research and Training Center, University of California, San

Diego, La Jolla,, CA, USA. [10]Center for Biomolecular Therapeutics, University of Maryland School of Medicine, Rockville, MD, USA

8:50 - 9:10am

204 Crystal Structures of 19b Fab Complexed with its HIV-1 Envelope Variable Region 3 Epitope Reveals Novel Interaction

Susan Fetics[1], Jared Lindenberger[1], Nathan Nicely[2], Chun-Hsing (Josh) Chen[2], Priyamvada Acharya[1]

[1]Duke University School of Medicine, Durham, NC, USA. [2]University of North Carolina at Chapel Hill, Chapel Hill, NC, USA

9:10 - 9:30am

116 Neutron crystallographic studies of crucial metabolic enzyme targeted by cancer

Victoria Drago[1], Roberts Phillips[2], Andrey Kovalevsky[3]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]University of Georgia Athens, Athens, GA, USA. [3]Oak Ridge National LaboratoryNeutron crystallographic studies of crucial metabolic enzyme targeted by cancer, Oak Ridge, TN, USA

9:30 - 9:50am

156 Unveiling the Molecular Interplay of VPS34 Inhibition by Novel Drug Targets: A Promising Approach for Tailored Cancer Therapeutics

Wisdom Abiodun, James Moody

Brigham Young University, Provo, Utah, USA

10:30 - 10:50am

170 A comprehensive strategy for quick determination of protein structures by MR-native SAD method

Miki Senda[1], Toshiya Senda[2]

[1]High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan. [2]High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan

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10:50 - 11:10am

158 Development of Constructs and Crystal Forms of HSP47 to Support Structure-Based Drug Design

Steven Sheriff[1], Kevin Kish[1], Stephen Cobell[1], Nicolas Szalpiel[1], Chunhong Yan[1], John Newitt[1], Jeffrey Tredup[1], Iyoncy Rodrigo[1], Elizabeth Tomasco[1], Mian Gao[1], Frank Marsilio[1], John Huagner[2], Dasa Lipovsek[2], Bi Deng[2], Patrick Bousquet[2], Holly Schmidt[2]

[1]Bristol-Myers Squibb Research and Development, Princeton, NJ, USA. [2]Bristol-Myers Squibb Research and Development, Cambridge, MA, USA

11:10 - 11:30am

123 Structural characterization of a novel class of antibacterials that target the lipopolysaccharide transporter MsbA in multidrug-resistant *Acinetobacter baumannii*

Daniel Klein[1], Hao Wang[1], Andrii Ishchenko[1], Jason Skudlarek[1], Pamela Shen[1], Liudmila Dzhekieva[1], Ronald Painter[1], Christina Chen[2], Marina Bukhtiyarova[1], Andrew Leithead[1], Rodger Tracy[1], Carolyn Bahnck-Teets[1], Alexei Buevich[1], Marc Labroli[1], Henry Lange[1], Wei Li[1], Paul Mann[1], Tao Meng[1], Helen Mitchell[1], Giovanna Scapin[2], Deyou Sha[1], Anthony Shaw[1], Ling Tong[1], Chengwei Wu[1], Zhe Wu[1], Randy Miller[1], Carl Balibar[1], Raheem Izzat[1], Scott Walker[1]

[1]Merck, West Point, PA, USA. [2]Merck, Rahway, NJ, USA

2.1.4 Algorithms & Computational Methods in CryoEM

8:30 - 11:30am Tuesday, 9th July, 2024
Evergreen C
Alexis Rohou, Joey Davis

Many challenges remain in the quest to fully unlock the potential of cryoEM for structural studies of biology. How can we resolve fine details of dynamic, flexible assemblies? What is the best way to study the structures of macromolecules in their native, cellular context? How can we control our instruments more efficiently for high-throughput, automated high-resolution imaging? What are the optimal methods for obtaining and validating accurate and reliable atomic models for molecules of interest? For these and many other challenges, the development of improved computational methods and algorithms remains a key stone of the field. This session will cover some of the latest computational work in cryoEM and cryoET.

8:30 - 9:00am

164 Cryo-EM Reconstruction and Interpretation: Leveraging Application-Specific Machine Learning

Dari Kimanius

CZII, Redwood City, CA, USA

9:00 - 9:30am

237 EMhub: a web platform for data management and on-the-fly processing in scientific facilities

Jose Miguel De la Rosa Trevin[1], Grigory Sharov[2], Stefan Fleischman[3], Dustin Morado[3], John Bollinger[1], Darcie Miller[1], Daniel Terry[1], Scott Blanchard[1], Israel Fernandez[4], Marta Carroni[3]

[1]St.Jude Children's Research Hospital, Memphis, TN, USA. [2]Laboratory of Molecular Biology, Cambridge, Cambridge, United Kingdom. [3]Science for Life Laboratory, Stockholm, Stockholm, Sweden. [4]Biofisika Institute, Bilbao, Bizkaia, Spain

9:30 - 10:00am

88 Improving Cryo-EM Experimental Data Fit with Automated Multiconformer Modeling for Proteins and Non-proteins

Stephanie Wankowicz, Jessica Flowers, Daniel Hogan, Ashraya Ravikumar, James Fraser

University of California San Francisco, San Francisco, CA, USA

10:30 - 10:50am

302 New Developments in Single Particle Cryo-EM Data Processing in CryoSPARC

Ali Punjani, CryoSPARC Team

Structura Biotechnology Inc., Toronto, ON, Canada

10:50 - 11:10am

304 Helicon: helical reconstruction from a single 2D image

Wen Jiang

Purdue University, West Lafayette, IN, USA

11:10 - 11:30am

336 CryoSTAR: Leveraging Structural Prior and Constraints for Cryo-EM Heterogeneous Reconstruction

Yilai Li[1], Yi Zhou[2], Jing Yuan[2], Fei Ye[2], Quanquan Gu[3]

[1]ByteDance Research, San Jose, CA, USA. [2]ByteDance Research, Shanghai, N/A, China.
[3]ByteDance Research, Los Angelos, CA, USA

2.1.5 Tips & Tricks for Modern Structural Methods

8:30 - 11:30am Tuesday, 9th July, 2024
Evergreen D
Lee Daniels, Susanna Huang

Have you collected data using a drone, solved a structure with your smartphone, or crystallized with sound waves from your guitar? We want to hear about it.

We've all heard about solvent evaporation and direct methods - what about the other tools you use? Let us know about finding phase transitions, wrangling twins, or paying for your research with Dogecoin. How did you get the difficult data from that diamond-anvil cell?

The Tips and Tricks session is your chance to share those quirky and ingenious tricks you use that you didn't learn from a lecture on structure factors.

Software - do you use an app or a program in a way that others should know about? Or maybe you've written one to share?

Structure solutions - how do you deal with tough problems? Twins? - solving, refining? Dealing with other tricky problems. What about electron diffraction?

Combining crystallography with other techniques - spectroscopy? microscopy? (drones?)

And we're not limited to crystallography - How do you organize your samples, your data, your results? How do you pay for your stuff?

What about presentations? Do you have a unique way to prepare slides, charts, movies?

And yes, we still want to hear about ways to grow crystals, handle and mount them, and make other measurements on them.

Tips and Tricks presentations will be short - possibly 5, maybe up to 15 minutes - so we get to enjoy as many of them as possible.

8:30 - 9:00am

125 High-Throughput Crystallisation of Organic Molecules on the Nanoscale - Successes, Challenges and Future Directions

Michael Hall

Newcastle University, Newcastle upon Tyne, Tyne and Wear, United Kingdom

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9:00 - 9:30am

220 APEX5 - Bridging the gap between X-ray - and Micro ED data

Michael Ruf

Bruker AXS, Madison, WI, USA

9:30 - 10:00am

252 On the Optimal Camera for Electron Diffraction Detection

Jung Cho, Matthew Mecklenburg

CNSI@UCLA, Los Angeles, CA, USA

10:30 - 11:00am

12 Program G1 – chemical formula analyzer

Ilia Guzei

University of Wisconsin-Madison, Madison, WI, USA

11:00 - 11:30am

67 The curious case of the unexpected neutron diffraction impurity

Brian Toby

Advanced Photon Source, Argonne Natl Lab, Lemon, IL, USA

2.1.6 Mathematical, Theoretical & Computational Crystallography

8:30 - 11:30am Tuesday, 9th July, 2024
Evergreen EF
Jared Allred, Branton Campbell

This session will focus on current developments in the theoretical and computational crystallography to the prediction, modeling, determination, and rational understanding of crystalline materials and their properties.

8:30 - 9:05am

234 Automatic structure classification – new tools and approaches

Peter Khalifah[1,2], Yusu Wang[3,2]

[1]Stony Brook University, Stony Brook, NY, USA. [2]Brookhaven National Laboratory, Upton, NY, USA. [3]Stony Brook, Stony Brook, NY, USA

9:05 - 9:30am

247 Discovering nonlinear optical crystals and predicting their THz spectra through data mining and DFT calculations

Sin Hang Ho, Stacey Smith, Jeremy Johnson, David Michaelis

Brigham Young University, Provo, Utah, USA

9:30 - 9:55am

211 A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Robert Hanson

St. Olaf College, Northfield, Minnesota, USA

10:30 - 11:05am

46 Learning many-body potential energy landscape for analysis of neutron scattering data

Gaurav Vishwakarma, Christina Hoffmann

Oak Ridge National Laboratory, Oak Ridge, TN, USA

11:05 - 11:30am

293 Large-angle rigid unit modes in crystalline frameworks

Branton J. Campbell, Bryce T. Eggers, Harold T. Stokes

Brigham Young University, Provo, Utah, USA

Exhibit Hall

10:00am - 12:00pm Tuesday, 9th July, 2024

PL1: Etter Award: Benjamin Frandsen

11:45am - 12:45pm Tuesday, 9th July, 2024
Evergreen A
Allen Oliver

Established in 2002, the Margaret C. Etter Early Career Award has recognized a long list of awardees who have exhibited outstanding achievement and exceptional potential in structural science research demonstrated by a scientist at an early stage of their independent career. This year Benjamin Frandsen will be receiving this award for his pioneering developments, both theoretical and experimental, of the novel magnetic pair distribution function (mPDF) method for studying short-range magnetic correlations in ordered and disordered magnetic systems, and for his outstanding leadership, mentorship and service to the community. We are thrilled to recognize the outstanding achievements of Benjamin Frandsen, while also spotlighting his remarkable leadership and dedication to the ACA community.

11:50am - 12:40pm

134 When the Tail Wags the Dog, aka Short-range Correlations with Long-range Implications: A Magnetic PDF Story

Benjamin A Frandsen

Brigham Young University Department of Physics and Astronomy, Provo, UT, USA

NIH/NIGMS Funding Opportunities

1:00 - 1:45pm Tuesday, 9th July, 2024
Evergreen B
Veronica Taylor, Thomas Cho

The National Institutes of Health's (NIH) mission is to seek fundamental knowledge about the nature and behavior of living systems and to apply that knowledge to enhance public health. In fulfilling its mission, the NIH offers an array of funding programs to extramural investigators at all career stages. The National Institute of General Medical Sciences (NIGMS) primarily supports basic research that increases the understanding of biological processes and lays the foundation for advances in disease diagnosis, treatment, and prevention. Although the majority of NIGMS awards are for investigator-initiated research projects (R01/R35), NIGMS also funds small business (SBIR/STTR) grants and research centers and resources. The latter include the National Centers for Cryoelectron Microscopy (R24) and Mature Synchrotron Resources for Structural Biology (P30). This session will provide an overview of the NIH grant process and highlight NIGMS funding opportunities that can benefit the ACA the Structural Science Society community.

418 A presentation about NIH/NIGMS funding opportunities

Thomas Cho

NIH/NIGMS, Bethesda, MD, USA

2.2.1 General Interest - Part 2

2:00 - 5:00pm Tuesday, 9th July, 2024
Conifer Ballroom
Tim Stachowski, Zhen Xu, Tori Drago

General Interest sessions are the forum for topics of broad interest to the structural science or for presentations that do not fit the specific theme of other sessions. All presentations are selected from submitted abstracts.

2:00 - 2:20pm

181 Structural basis of negative feedback regulation in mevalonate kinase inhibition

Yan Kung

Bryn Mawr College, Bryn Mawr, PA, USA

2:20 - 2:40pm

209 Key structural role of a conserved cis-proline revealed by the P285S variant of soybean serine hydroxymethyltansferase 8

Vindya Samarakoon[1], Luckio F. Owuocha[2], Jamie Hammond[2], Melissa G. Mitchum[3], Lesa J. Beamer[1,2]

[1]Department of Chemistry, University of Missouri, Columbia, MO, USA. [2]Department of Biochemistry, University of Missouri, Columbia, MO, USA. [3]Department of Plant Pathology and Institute of Plant Breeding, Genetics and Genomics, University of Georgia, Athens, GA, USA

2:40 - 3:00pm

26 ***Structure of saguaro cactus virus 3' translational enhancer mimics 5' cap for eIF4E binding***

Manju Ojha[1], Jeff Vogt[2], Naba Krishna Das[1], Emily Redmond[1], Karndeep Singh[3], Hasan Al Banna[1], Tasnia Sadat[1], Deepak Koirala[1]

[1]University of Maryland Baltimore County, Baltimore, MD, USA. [2]Johns Hopkins, Baltimore, MD, USA. [3]University of Maryland Baltimore County, HHMI, Baltimore, MD, USA

3:30 - 3:55pm

317 Cryo-EM Determines the Epitope of a 28 kD Viral Protease in Complex with an Antibody Fragment

Marcell Zimanyi[1], Kaitlin Hulce[2], Charles Craik[1], Yifan Cheng[1]

[1]University of California San Francisco, San Francisco, CA, USA. [2]University of Washington, Seattle, WA, USA

3:55 - 4:15pm

270 Sub-tomogram averaging of structural proteins from respiratory syncytial virus released from cells grown and infected on grids reveals molecular organization of filamentous virions

Bryan S Sibert[1,2,3], Joseph Y Kim[1,4], Jie E Yang[1,2,3], Zunlong Ke[5], Elizabeth R Wright[1,2,3,6]

[1]Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [2]Cryo-Electron Microscopy Research Center, Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [3]Midwest Center for Cryo-Electron Tomography, Department of Biochemistry, University of Wisconsin, Madison, WI, USA. [4]Department of Chemistry, University of Wisconsin, Madison, WI, USA. [5]Department of Molecular Biosciences, University of Texas at Austin, Austin, TX, USA. [6]Morgridge Institute for Research, Madison, WI, USA

4:15 - 4:35pm

235 Cryo-EM reveals a bi-copper cluster coordinating asymmetric electron transfer in the nitrogenase-like DPOR complex

Rajnandani Kashyap[1], Jaigeeth Deveryshetty[1], Natalie Walsh[1], Brian Bennett[2], Edwin Antony[1]

[1]Saint Louis University, St Louis, MO, USA. [2]Marquette University, Milwaukee, WI, USA

4:35 - 5:00pm

228 The Single Particle CryoEM Structure of Bovine Liver Catalase from Lyophilized Powder

Jonathan Herrmann, Helen Donelick, Ayala Carl, John Spear

Thermo Fisher Scientific, Hillsboro, OR, USA

2.2.2 Light Sources Through the Decades - Part 2

2:00 - 5:00pm Tuesday, 9th July, 2024
Evergreen A
Marco Mazzorana, Cora Lind-Kovacs

2:00 - 2:30pm

216 The New Era of Structural Science

Uta Ruett

Argonne National Laboratory, Lemont, IL, USA

2:30 - 3:00pm

283 The renewed GM/CA@APS Structural Biology Facility and APS-Upgrade

Robert Fischetti[1], Michael Becker[1], Stephen Corcoran[1], Dale Ferguson[1], Mark Hilgart[1], David Kissick[1], Oleg Makarov[1], Craig Ogata[1], Sergey Stepanov[1], Nagarajan Venugopalan[1], Qingping Xu[1], Shenglan Xu[1], Janet Smith[2]

[1]Argonne National Laboratory, Lemont, Il, USA. [2]University of Michigan, Ann Arbor, Mi, USA

3:30 - 4:00pm

127 The Upgrade of the Macromolecular Crystallography Beamline X06DA-PXIII at SLS 2.0

Vincent Olieric, Benedikt Rösner, Dominik Buntschu, Wayne Glettig, Tomislav Marijolovic, Istvan Mohacsi, Kate Smith, Filip Leonarski, Ezequiel Panepucci, Chia-Ying Huang, Guillaume Gotthard, Takashi Tomizaki, Anuschka Pauluhn, Katherine McAuley, Meitian Wang

Paul Scherrer Institut, Villigen PSI, AG, Switzerland

4:00 - 4:30pm

276 SERCAT II - the next generation

John Rose[1,2], John Chrzas[1,2], James Fait[1,2], Zheng-Qing "Albert" FU[1,2], Zhongmin Jin[1,2], Michael Molitsky[1,2], Rod Salazar[1,2], Unmesh Chinte[1,2], Palani Kandavelu[1,2]

[1]University of Georgia, Athens, GA, USA. [2]SER-CAT, APS, Lemont, IL, USA

4:30 - 5:00pm

159 Massive Compression for High Data Rate Macromolecular Crystallography (HDRMX): Impact on Diffraction Data and Subsequent Structural Analysis

Herbert J Bernstein[1], Alexei Soares[2], Kimberly Horvat[3], Jean Jakoncic[2]

[1]Fresh Pond Research Institute, New York, NY, USA. [2]Brookhaven National Laboratory, Upton, NY, USA. [3]Stony Brook University, Stony Brook, NY, USA

2.2.3 Structural Biology in Pharma/Biotech - Part 2

2:00 - 5:00pm Tuesday, 9th July, 2024
Evergreen B
Sandra Gabelli, Elizabeth Sprague

A full-day session dedicated to exploring various topics in Structural Biology in Pharma/Biotech. We invite submissions on any topic related to the industrial application of structural biology, including but not limited to: vaccines, CART-T, TPD/TPS glues, macrocyclic peptides, induced proximity, and FBDD. Additionally, we encourage presentations that utilize a variety of techniques such as x-ray, NMR, EM, in silico, and biophysics. Technology or methods development in these areas is also of interest. Accepted abstracts will be grouped and assigned to a specific session.

2:00 - 2:20pm

320 Disulfide constrained Fabs overcome target size limitation for high-resolution single particle cryoEM

Jawahar Sudhamsu[1], Jennifer Kung[1], Matthew Johnson[1], Christine Jao[1], Christopher Arthur[2], Dimitry Tegunov[1], Alexis Rohou[1]

[1]Genentech Inc., South San Francisco, CA, USA. [2]Altos Labs, South San Francisco, CA, USA

2:20 - 2:40pm

279 High throughput mutagenesis to promote oligomerization to access cryo EM: a case study for HSD17b13

Jill Chrencik[1], Sandra Gabelli[2]

[1]Merck, South San Francisco, CA, USA. [2]Merck, West Point, PA, USA

2:40 - 3:00pm

229 Novel Fragment Inhibitors of PYCR1 from Docking-Guided X-ray Crystallography

Kaylen Meeks[1], Juan Ji[1], Mykola Protopopov[2], Olga Tarkhanova[2], Yurii Moroz[2,3], John Tanner[1]

[1]University of Missouri, Columbia, Missouri, USA. [2]Chemspace LLC, Kyïv, 02094, Ukraine. [3]Taras Shevchenko National University of Kyïv, Kyïv, 01601, Ukraine

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3:30 - 3:50pm

61 Using the Quantum Interface in Phenix to improve macromolecular model and ligand structures

Nigel Moriarty[1], Jonathan Moussa[2], Paul Adams[1,3]

[1]Lawrence Berkeley Lab, Berkeley, CA, USA. [2]Virginia Tech, Blacksberg, VT, USA. [3]University of California Berkeley, Berkeley, CA, USA

3:50 - 4:10pm

162 CRAFT (CENTER FOR THE RESEARCH AND ADVANCEMENT IN FRAGMENTS AND MOLECULAR TARGETS) : A BRAZILIAN CENTER FOR DRUG DISCOVERY

Maria Cristina Nonato[1,2], Flavio da Silva Emery[1,2], Carolina Horta Andrade[1,3]

[1]Center for Research and Advancement of Fragments and Molecular Targets (CRAFT), Ribeirão Preto, SP, Brazil. [2]University of São Paulo, School of Pharmaceutical Sciences, Ribeirão Preto, SP, Brazil. [3]Federal University of Goiás, School of Pharmacy, Ribeirão Preto, SP, Brazil

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4:10 - 4:30pm

4 Speeding up drug discovery with high-quality and high-reliability crystallography-based library screening

Debanu Das

Accelero Biostructures Inc, San Carlos, CA, USA

4:30 - 4:50pm

44 Branched chain ketoacid dehydrogenase kinase inhibitors: from fragments to clinical candidate

Shenping Liu

Pfizer Inc, Groton, CT, USA

2.2.4 Symmetry and Emergent Orders in Quantum and Strongly Correlated Materials

2:00 - 5:00pm Tuesday, 9th July, 2024
Evergreen C
Yu Li, Keith Taddei

This session will focus on topological, quantum, and correlated electron materials broadly, emphasizing the effects of structure and symmetries in generating novel properties and emergent phases. Example topics include time reversal symmetry breaking and magnetism; altermagnetism; symmetry protected topological phases; unconventional superconductivity; quantum spin liquids; Kagome/triangular/honeycomb lattices; and skyrmion materials.

2:00 - 2:30pm

101 Novel Rare-Earth i-MAX Phases: From Synthesis to Magnetic Properties and Beyond toMXenes

Binod Rai[1], Alex Bretana[1], Tucker Koenig[1], Ram Rai[2], Bishnu Bastakoti[3], Christopher Mizzi[4], Boris Maiorov[4], Bhoj Gautam[5]

[1]Savannah River National Laboratory, Aiken, SC, USA. [2]SUNY Buffalo State, Buffalo, NY, USA. [3]North Carolina A&T State University, Greensboro, NC, USA. [4]Los Alamos National Laboratory, Los Alamos, NM, USA. [5]Fayetteville State University, Fayetteville, NC, USA

2:30 - 3:00pm

206 Diffuse neutron scattering on geometrically frustrated Bi2(Fe1-xGax)4O9

Yu Li

Argonne National Laboratory, Lemont, IL, USA

3:30 - 3:50pm

219 Structure-Property Relationship in the Kagomé Net Intermetallic Co_3Ge_2Sb

Nolan Stager, Jared Allred, Sachini Lokusuriya

University of Alabama, Tuscaloosa, Al, USA

3:50 - 4:10pm

292 Investigating phase coexistence and local structure in $MoTe_2$ using synchrotron XRD and pair distribution function

Sumit Khadka[1,2], Byron Freelon[1,2], Leighhane Gallington[3]

[1]University of Houston, Houston, TX, USA. [2]Texas Center for Superconductivity, Houston, TX, USA. [3]Advanced Photon Source (X-ray Science Division), Lemont, IL, USA

4:10 - 4:30pm

82 Redox-coupled structural distortions in the quasi-1-dimensional $Au_2M_{1-x}P_2$ system

Scott Lee[1], Joseph Stiles[1], Jonathan Van Buskirk[2], Fang Yuan[1], Fatmagül Katmer[1], Stephanie Dulovic[1], Tieyan Chang[3,4], Daniel Fredrickson[2], Yu-Sheng Chen[3,4], Leslie Schoop[1]

[1]Princeton University, Princeton, NJ, USA. [2]University of Wisconsin, Madison, WI, USA. [3]Argonne National Lab, Lemont, IL, USA. [4]University of Chicago, Chicago, IL, USA

4:30 - 4:50pm

255 Interesting magnetic properties of a dubious Weyl semimetal

Keith Taddei[1], Daniel Phelan[1], Duminda Sanjeewa[2], Sanjaya Ranmohotti[3]

[1]Argonne National Laboratory, Lemont, IL, USA. [2]University of Missouri, Columbia, MO, USA. [3]Governors State University, University Park, IL, USA

2.2.5 Using Microed at Your Institution: How Microed &Cryo-EM Can Coexist

2:00 - 5:00pm Tuesday, 9th July, 2024
Evergreen D
Brent Nannenga, Tamir Gonen

The use of MicroED is expanding with many institutions adding the technique to their suite of structure determination methods. MicroED uses much of the same infrastructure as other cryo-EM modalities, therefore many user facilities can offer MicroED along side single-particle cryo-EM and cryo-ET. This session will focus experiences integrating and applying MicroED, as well as best practices to ensure how all cryo-EM methods can coexist.

2:00 - 2:15pm

226 Establishing a MicroED workflow at the Hauptman-Woodward Institute

Katherine A. Spoth, Gabrielle R. Budziszewski, M. Elizabeth Snell, Christopher S. Campomizzi, Miranda L. Lynch, Devrim Acehan, Sarah E. J. Bowman

Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA

2:15 - 2:30pm

151 Big Sky Little Crystals— A MicroED Collaboration Between Core Facilities at Montana State University and the University of Montana

Daniel Decato

University of Montana, Missoula, Montana, USA

2:30 - 2:45pm

199 Setup and operation of 3DED/microED experiments at KEK and Tsukuba Univ.

Naruhiko Adachi[1,2], Yusuke Yamada[2], Kenji Iwasaki[1], Toshiya Senda[2]

[1]The University of Tsukuba, Tsukuba, Ibaraki, Japan. [2]KEK, Tsukuba, Ibaraki, Japan

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2:45 - 3:00pm

305 Integrating MicroED and Other Cryo-EM Modalities at UCLA

Ampon Saeher, Tamir Gonen

UCLA, LA, CA, USA

3:30 - 3:45pm

260 Access and Experiments with MicroED at Yale University for Biomaterials Characterization

Charles Lomba[1], Brandon Mercado[1], Alison Sweeney[2]

[1]Yale University, New Haven, CT, USA. [2]Ya, Yale University, CT, USA

3:45 - 4:00pm

75 FIB milling cells and crystals, not too separate realities

William Nicolas, Tamir Gonen

HHMI, Los Angeles, CA, USA

4:00 - 4:15pm

258 Transforming a cryo-TEM into a multi-faceted tool: Electron Diffraction at the Simons Electron Microscopy Center

Christina M Zimanyi[1], Hui Wei[1,2], Lambertus M Alink[1], Edward T Eng[1], Alex de Marco[1]

[1]New York Structural Biology Center, New York, NY, USA. [2]Rutgers New Jersey Medical School, Newark, NJ, USA

4:15 - 4:30pm

316 UC Irvine Materials Research Institute – Expanding a Materials Facility with Biological CryoEM and MicroED

Shane Gonen

University of California, Irvine, Irvine, CA, USA

2.2.6 Engaging Students Part 1

2:00 - 5:00pm Tuesday, 9th July, 2024
Evergreen EF
Yinka Olatunji-Ojo, Joe Tanski

This session is focused on how to effectively engage students at any level with crystallography in teaching and research. Specific topics may include student training and mentoring in research that involves crystallography, pedagogy and building crystallography teaching infrastructure, strategies for faculty professional success in research involving crystallography, effective involvement of students at synchrotron facilities, and approaches towards instrument acquisition and maintaining resources for engaging students with crystallography.

2:00 - 2:20pm

312 Crystallizing Student-Interest in Crystallography

Susanna Huang[1,2,3], Selina Huang[2,3]

[1]Georgia Institute of Technology, Atlanta, GA, USA. [2]SeNA Research Institute, Atlanta, GA, USA. [3]STARS crystallography research, Atlanta, GA, USA

2:20 - 2:40pm

207 Using the Cambridge Structural Database for Teaching Crystallography

Diane Dickie

University of Virginia, Charlottesville, VA, USA

2:40 - 3:00pm

48 Post-COVID Extension of an Online Crystallography School

Joseph Ferrara[1], Robert Bücker[2], Mark Del Campo[1], Lee Daniels[1], Christian Göb[2], Emilia Götz[2], PIerre Le Maguerès[1], Horst Puschmann[3], Mathias Meyer[4], Christian Schürmann[2], Khai-Nghi Truong[2], Jakub Wojciechowski[2], Fraser White[2]

[1]Rigaku Americas, The Woodlands, TX, USA. [2]Rigaku Europe SE, Neu-Isenburg, Hesse, Germany. [3]OlexSys, Durham, Durham, United Kingdom. [4]Rigaku Polska, Wrocław, Silesia, Poland

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3:30 - 3:55pm

259 An online Protein X-ray crystallography course engaging undergraduate students in structure building and refinement

Christine Phillips-Piro

Franklin & Marshall College, Lancaster, PA, USA

3:55 - 4:20pm

50 Teaching crystallography in virtual reality environments

Brandon Mercado

Yale University, New Haven, CT, USA

4:20 - 4:45pm

182 Using Jmol to engage students and teach crystallography and crystallographic symmetry

Dean Johnston[1], Robert Hanson[2]

[1]Otterbein University, Westerville, OH, USA. [2]St. Olaf College, Northfield, MN, USA

Exhibit Hall

2:00 - 7:30pm Tuesday, 9th July, 2024

PS2: Poster Session #2

5:00 - 7:30pm Tuesday, 9th July, 2024
Atrium

327 Porous protein microcrystals for delivery of nucleic acids

Alec Jones[1], Anika O'Brian[1], Katherine Horak[2], Christopher Snow[1]

[1]Colorado State University, Fort Collins, CO, USA. [2]USDA-APHIS NWRC, Fort Collins, CO, USA

413 Synthesis and Characterization of Photomechanical Azobenzene Cocrystals

Nikki Williams[1], David McGee[1], Amy Sarjeant[2], Heba Abourahma[1]

[1]The College of New Jersey, Ewing, NJ, USA. [2]Bristol Myers Squibb, New Brunswick, New Jersey, USA

409 Puzzling three-component disorder from unprecedented reaction

Nobuyuki Yamamoto, Austin Chivington, Sammie Squire, Jeremy Smith

Indiana University, Bloomington, Bloomington, IN, USA

397 Resolving polymer flipping in TELSAM-facilitated protein crystals using magneto crystallography

James Moody, Maria Pedroza, Alihi Keliiliki

Brigham Young University, Provo, Utah, USA

407 Opening Doors in Protein Crystallization: TELSAM with two pH Triggers

Miles Bradford, Jacob Averett, Blake Averett, Dalton Hansen, James Moody

Brigham Young University, Provo, UT, USA

375 Improving 1TEL-DARPin Crystallization via Linker Diversity Optimization for Enhanced Crystal Quality and Diffraction Data

James Moody, Maria Pedroza, Ethan Noakes

Brigham Young University, Provo, Utah, USA

350 What is the best target protein density for TELSAM fusion crystallization?

Kyle Ludlow, James Moody

Brigham Young University, Provo, Utah, USA

401 Probing the function and structure of SwrD, a potential flagellar motor power enhancer

Dhruva Nair, Brian Crane

Cornell University, Ithaca, NY, USA

380 **Robust error calibration for serial crystallography**

David Mittan-Moreau, Daniel Paley, Nicholas Sauter, Aaron Brewster

Lawrence Berkeley National Lab, Berkeley, Ca, USA

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414 **Structural and biochemical insights into D-cycloserine tolerance in *Staphylococcus aureus***

Yahani Jayasinghe, Sasmita Panda, Vinai Thomas, Donald Ronning

University of Nebraska Medical Center, Omaha, Nebraska, USA

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389 **Structural and Functional Analysis of Sporulation and Germination in Bacterial Endospores**

Doyeon Kim, Dukwon Lee, Yeongjin Baek, Jinwook Lee, Nam-Chul Ha

Seoul National University, Seoul, Gwanak District, Korea, Republic of

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406 **Towards the spatial resolution of photosystem II charge states from XFEL diffraction data**

Daniel Tchon[1], Johannes Blaschke[2], Vidya Ganapati[1], Daniel Paley[1], Billy Poon[1], Felix Wittwer[2], Iris Young[1], Aaron Brewster[1], Junko Yano[1], Jan Kern[1], Vittal Yachandra[1], Nicholas Sauter[1]

[1]Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging, Berkeley, CA, USA. [2]Lawrence Berkeley National Laboratory, National Energy Research Scientific Center, Berkeley, CA, USA

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78 **Determining the Mechanism of DJ-1 Using Mix-and-Inject Synchrotron Serial Crystallography**

Cole Dolamore[1], Kara Zielinski[2], Kevin Dalton[3], Stephen Meisburger[4], John Termini[5], Nathan Smith[1], Robert Henning[6], Vukica Srajer[6], Doeke Hekstra[3], Lois Pollack[2], Mark Wilson[1]

[1]University of Nebraska - Lincoln, Lincoln, NE, USA. [2]Cornell University, Ithaca, NY, USA. [3]Harvard University, Cambridge, MA, USA. [4]Cornell High Energy Synchrotron Source, Ithaca, NY, USA.

[5]Beckman Research Institute, City of Hope, CA, USA. [6]Argonne National Laboratory (BioCARS), Lemont, IL, USA

372 Probing an enzyme active site with time-resolved serial femtosecond crystallography by a liquid injector and a belt system

Fangjia Luo[1], Michihiro Sugahara[2], Tetsunari Kimura[3], Takanori Nakane[4], Jungmin Kang[2], Nipawan Nuemket[1,2], Kensuke Tono[1,2], Makina Yabashi[1,2], So Iwata[5], Eriko Nango[6]

[1]Japan Synchrotron Radiation Research Institute (JASRI), Sayo, Hyogo, Japan. [2]RIKEN Harima, Sayo, Hyogo, Japan. [3]Kobe University, Kobe, Hyogo, Japan. [4]Osaka University, Osaka, Osaka, Japan. [5]Kyoto University, Kyoto, Kyoto, Japan. [6]Tohoku University, Sendai, Miyagi, Japan

39 Mapping allosteric rewiring across a family of dynamic tyrosine phosphatases

Shivani Sharma, Akshay Raju, Daniel A Keedy

City University of New York, New York, NY, USA

363 Exploring the molecular mechanisms of temperature sensing by Cdc2-like-Kinases.

Luisa R. Garcia Michel[1], Gyselle A. Godinez Castillo[2], Miguel Estrada Caballero[1], Felizardo Salazar[1], Younghwan Kwak[1], Gordon Bennett[1], Michael Thompson[1]

[1]University of California, Merced, Merced, CA, USA. [2]Instituto Politecnico Nacional, Ciudad de Mexico, Estado de Mexico, Mexico

387 Automated vitrification with self-wicking grids may limit potential preferred orientation of CRL5-PCMTD1, a putative cullin-RING ligase, during cryoEM sample preparation

Eric Pang, Steve Clarke, Jose Rodriguez

University of California, Los Angeles, Los Angeles, California, USA

384 Synthesis and Reactivity of Late Transition Metal–Sb Complexes

Christopher Webber, Fanji Kong, Diane Dickie, Brent Gunnoe

University of Virginia, Charlottesville, VA, USA

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366 Using Microcrystal Electron Diffraction (MicroED/3DED) for Small Molecule Structure Determination and Beyond at The University of Texas at Austin

Gabriella Ruiz

University of Texas at Austin, Austin, TX, USA

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374 Crystal Growth and Crystallography of a Complex Transition Metal Oxide

Paul Cardon[1], Evan Crites[2], Satya Kushwaha[2], Huiwen Ji[1]

[1]University of Utah, Salt Lake City, Utah, USA. [2]Johns Hopkins University, Baltimore, Maryland, USA

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11 Crystal Structures of Large-Volume Commercial Pharmaceuticals

James Kaduk[1], Tawnee Ens[1], Anja Dosen[2], Thomas Blanton[2]

[1]North Central College, Naperville, IL, USA. [2]ICDD, Newtown Square, PA, USA

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358 Molecular Interplay of VPS34 Inhibition by Novel Drug Targets: A Promising Approach for Tailored Cancer Therapeutics

Wisdom Abiodun

Brigham Young University, Provo, Utah, USA

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356 Pink and blue materials with olivine solid solutions and pink diopside solid solutions: towards more sustainable pigments

Santiago Garcia-Granda[1], M. A. Tena[2], Mohammed S. M. Abdelbaky[3], Camino Trobajo[1], José R. García[1]

[1]University Oviedo, Oviedo, Asturias, Spain. [2]University of Jaume I, Castellon de la Plana, Valencia, Spain. [3]University of Salamanca, Salamanca, Salamanca, Spain

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415 TELSAM-DARPin protein complexes may exhibit partial molecule exclusion when in complex with target proteins

Blake Averett

Brigham Young University, Provo, Utah, USA

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77 Accelerating NLRP3 drug discovery by leveraging a multipronged structural biophysics strategy

Jill Chrencik

Merck, South San Francisco, CA, USA

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386 The D Gene in CDR H3 Determines a Public Class of Human Antibodies to SARS-CoV-2

Meng Yuan, Ian Wilson

The Scripps Research Institute, La Jolla, California, USA

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186 Structural insights into Polymorphic toxin –Immunity pair system of *Bacillus subtilis*.Charandeep Singh, Soni Kaundal, Amar Deep, Rishita Rohilla, Maheshwaran Velusamy, Krishan Gopal Thakur**Council of Scientifc and Industrial Research, Institute of Microbial Technology, Chandigarh, India, 160036Email: Charaandeep@gmail.com*

Charandeep Singh

CSIR - Institute of Microbial Technology, Chandigarh, Chandigarh, India

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355 Novel Fragment Inhibitors of PYCR1 from Docking-Guided X-ray Crystallography

Kaylen Meeks[1], Juan Ji[1], Mykola Protopopov[2], Olga Tarkhanova[2], Yurii Moroz[2,3], John Tanner[1]

[1]University of Missouri, Columbia, MO, USA. [2]Chemspace LLC, Kyïv, 02094, Ukraine. [3]Taras Shevchenko National University of Kyïv, Kyïv, 01601, Ukraine

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408 Exploring the Crystal Structure of tRNA Methyltransferase from Mycobacterium abscessus

Giavana Prucha[1], Vivian Stojanoff[2], Maham Ismail[3]

[1]NYIT College of Osteopathic Medicine, Old Westbury, New York, USA. [2]Brookhaven National Laboratory, Upton, New York, USA. [3]Stony Brook University, Stony Brook, New York, USA

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391 DNA Supercoiling is Required for Efficient Formation of R-loops

Taylor White, Charles Bou-Nader

Emory University, Atlanta, GA, USA

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51 Bridging the Gap: Early Exposure to Crystallography in Undergraduate Education

Alexis Paskach, Joshua James

University of Alabama in Huntsville, Huntsville, AL, USA

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432 Using structure and informatics to probe the mechanism of enzymes in the flavin amine oxidase superfamily

Kristin Hughes[1], Riley Osadchey Brown[1], Sydney Brender[2], Adrian Whitty[1], Qiang Cui[1], Bruce Palfey[2], Karen Allen[1]

[1]Boston University, Boston, MA, USA. [2]University of Michigan, Ann Arbor, MI, USA

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436 Over-Stoichiometric Metastabilization of Manganese-Based Cation-Disordered Rock Salts

You Wang, Wonu Choe, Dongchang Chen

University of New Mexico, Albuquerque, New Mexico, USA

430 Structure and mechanism of the GO DNA repair enzyme MutY from bacteria and its human homolog MUTYH

Martin Horvath[1], L. Peyton Russelburg[1,2], Merve Demir[3,4], Melody Malek[3], Carlos Trasviña-Arenas[3,5], Sheila David[3]

[1]University of Utah, Salt Lake City, UT, USA. [2]BioRad, Hercules, CA, USA. [3]University of California, Davis, CA, USA. [4]Sanford Burnham Prebys Medical Discovery Institute, San Diego, CA, USA. [5]Cenvistav, Mexico City, Ciudad de México, Mexico

447 Neutron Protein Crystallography at Oak Ridge National Laboratory

Victoria N Drago, Dominic Giuliano, Andrey Kovalevsky, Flora Meilleur, Dean A A. Myles, Josh Pierce

Oak Ridge National Lab, Oak Ridge, TN, USA

ACA Fellows Reception - Invite Only

6:00 - 8:00pm Tuesday, 9th July, 2024
Cottonwood

2.3.1 Career Odysseys

7:30 - 9:30pm Tuesday, 9th July, 2024
Evergreen A
Melanie Adams Cioaba, Eddie Pryor, Kristofer Gonzalez-DeWhitt

This session will target students, postdocs and early career scientists seeking to learn more about a variety of career paths. We will feature speakers from academia, industry, and government serving in a variety of roles. This will be an interactive session, with audience participation encouraged.

7:30 - 7:40pm

180 My U-turn: a journey from academic medicine to industry

Sandra Gabelli

Merck & Co, West Point, PA, USA

7:40 - 7:50pm

277 My academic career journey in structural science and engineering

Brent Nannenga

Arizona State University, Tempe, AZ, USA

7:50 - 8:00pm

332 Cryo-EM in academia, nonprofits, startups, and biotech

Caleigh Azumaya

Genentech, South San Francisco, CA, USA

8:00 - 8:10pm

326 Photon to Electron - Journey of a Forever Student!

Surajit Banerjee

Thermo Fisher Scientific, Hillsboro, OR, USA

8:10 - 8:20pm

346 From crystallography to alt-ac drug discovery to NIH

Leigh Allen

National Institutes of Health, Bethesda, MD, USA

8:20 - 8:30pm

344 Starting and Growing a Gene-to-Structure Services Company

Joshua Carter

Helix BioStructures, LLC., Indianapolis, IN, USA

Registration Desk

7:00am - 5:00pm Wednesday, 10th July, 2024
Rocky Foyer - Pint Brothers BY

Speaker Ready Room

7:00am - 5:00pm Wednesday, 10th July, 2024
Spruce 2

For presenters, the ACA offers a dedicated space where you can review and rehearse your materials to ensure everything is in order before your presentation. We highly encourage presenters to utilize this resource to ensure their presentations are ready and polished.

3.1.1 Engaging Students with Crystallography Part 2

8:30 - 11:30am Wednesday, 10th July, 2024
Evergreen EF
Yinka Olatunji-Ojo, Joe Tanski

This session is focused on how to effectively engage students at any level with crystallography in teaching and research. Specific topics may include student training and mentoring in research that involves crystallography, pedagogy and building crystallography teaching infrastructure, strategies for faculty professional success in research involving crystallography, effective involvement of students at synchrotron facilities, and approaches towards instrument acquisition and maintaining resources for engaging students with crystallography.

8:30 - 8:55am

223 CCDC at Crystallographic Schools: Training Crystallographers with a Database of >1.2 million Structures

Jeff Lengyel[1], Yinka Olatunji-Ojo[1], Ilaria Gimondi[2], Suzanna Ward[2], Andrew Peel[2]

[1]CCDC Inc, Boston, MA, USA. [2]CCDC, Cambridge, Cambridgeshire, United Kingdom

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8:55 - 9:20am

202 ACA Video Library (AVL) Update.

Allen Oliver[1], Alain Beauparlant[2], Karen Glass[3], Matthew Brown[4], Tiffany Kinnibrugh[5], Yinka Olatunji-Ojo[6], Charlotte Stern[7], Kristina Vitale[8], Kristin Stevens[8]

[1]University of Notre Dame, Notre Dame, IN, USA. [2]East Tennessee State University, Johnson City, TN, USA. [3]University of Vermont, Burlington, VT, USA. [4]University of British Columbia, Kelowna, BC, Canada. [5]Argonne National Laboratory, Chicago, IL, USA. [6]Cambridge Crystallographic Data Center, Oakland, CA, USA. [7]Northwestern University, Evanston, IL, USA. [8]ACA HQ, Buffalo, NY, USA

9:20 - 9:45am

30 Establishing shared standards for cryoEM training curricula that is honored across multiple centers

Edward Eng, Mahira Aragon, Dianne Carpen, Cathleen Castello, Eugene Chua, Alex de Marco, Charlie Dubbeldam, Jeffrey Kieft, Elina Kopylov, Aaron Owji, Christina Zimanyi

New York Structural Biology Center, New York, NY, USA

10:30 - 10:50am

313 Unveiling the Inherent Beauty of Crystallography to Undergraduate Students

Susanna Huang

Georgia Institute of Technology, Atlanta, GA, USA. STARS crystallography research, Atlanta, GA, USA

10:50 - 11:10am

113 Broader Impacts of Women in Crystallography

Bart Kahr

New York University, NYC, NY, USA

11:10 - 11:30am

301 The Cambridge Structural Database: An Outstanding Resource for Enhancing the Undergraduate Learning Experience

Heba Abourahma

The College of New Jersey, Ewing, NJ, USA

3.1.2 Structure of Nucleic Acids - Part 1: CryoEM

8:30 - 11:30am Wednesday, 10th July, 2024
Evergreen A
Yuan He, Melanie Ohi

RNA, DNA, and nucleic acid-protein complexes remain challenging targets for structural biology. Nucleic acids are often structurally flexible even when complexed to their protein partners and it can be difficult to purify large enough quantities of stable nucleic acids or nucleic-protein complexes for conventional structural approaches such as NMR or X-ray crystallography. This session focuses on presenting approaches and techniques for using single particle cryo-EM to determine structures of dynamic nucleic acids and nucleic-protein complexes.

8:30 - 8:55am

86 Structural mechanisms of DNA priming by polymerase α–primase

Elwood Mullins[1], Lauren Salay[1], Clarissa Durie[2], Noah Bradley[1], Jane Jackman[3], Melani Ohi[4], Walter Chazin[1], Brandt Eichman[1]

[1]Vanderbilt University, Nashville, TN, USA. [2]University of Missouri, Columbia, MO, USA. [3]The Ohio State University, Columbus, OH, USA. [4]University of Michigan, Ann Arbor, MI, USA

8:55 - 9:15am

321 Cryo-EM Structures of Group II Intron Ribonucleoprotein Complexes

Sarah Starcovic, Evan Cramer, Aaron Robart

West Virginia University, Morgantown, WV, USA

9:15 - 9:35am

174 Conformations of a conserved arginine-rich bridge helix of Cas9 and Cas12a regulate off-target DNA cleavage

Rakhi Rajan, Chhandosee Ganguly, Lindsie Martin, Sydney Newsom, Leonard Thomas

University of Oklahoma, Norman, OK, USA

9:35 - 10:00am

212 Structural biology of telomerase mechanism and interactions at telomeres

Juli Feigon

University of California Los Angeles, Los Angeles, CA, USA

10:30 - 10:50am

141 Understanding alternative splicing regulation using yeast U1 snRNP

Shasha Shi, Collette Wright, Rui Zhao

University of Colorado Anschutz Medical Campus, Aurora, CO, USA

10:50 - 11:10am

289 Structural Study of HIV-1 Reverse Transcription Initiation

Yihua Li[1], Gabrielle Law[2], Samuel Carlson[2], Janet Smith[1], Victoria D'Souza[2], Melanie Ohi[1]

[1]University of Michigan, Ann Arbor, MI, USA. [2]Harvard University, Cambridge, MA, USA

11:10 - 11:30am

308 Single-particle cryo-EM reveals a novel form of viral 3D tRNA mimicry

Steve Bonilla

Rockefeller University, New York, NY, USA

3.1.3 Flexibility, Dynamics, And The Secret Lives Of Proteins Part 1

8:30 - 11:30am Wednesday, 10th July, 2024
Evergreen B
Marcus Fischer, Tim Stachowski
Proteins are notorious shapeshifters that change conformations in response to environmental cues like temperature, pH, and ligand binding. This flexibility often underpins biological processes like enzyme catalysis and signal transduction. Recent advances in technologies and modeling algorithms move beyond understanding protein structures as static images and closer to generating molecular movies of proteins throughout their active lifecycles. In turn, these experiments can reveal new opportunities to modulate protein function for therapeutics and biology. This session will focus on emerging methods for exploring protein flexibility, examples where flexibility reveals functional insights, and applications in modulating proteins and drug design.

8:30 - 9:00am

230 Visualization of transient states and molecular motions in the catalytic cycle of the proline catabolic bifunctional enzyme Proline Utilization A from kinetic crystallography and molecular dynamics simulations

David Buckley, John Tanner

University of Missouri, Columbia, Missouri, USA

9:00 - 9:30am

139 The Role of Structural Dynamics in the Regulation of Aspartate Transcarbamoylase Uncovered by SAXS and Cryo-Electron Microscopy

Robert Miller[1], Michael Patterson[1], Nozomi Ando[2]

[1]Cornell Univeristy, Ithaca, NY, USA. [2]Cornell University, Ithaca, NY, USA

9:30 - 10:00am

60 Structural insights into GrpEL1-mediated nucleotide and substrate release of mitochondrial Hsp70

Mark Herzik, Marc Morizono, Kelly McGuire, Natalie Birouty

University of California, San Diego, La Jolla, CA, USA

10:30 - 11:00am

187 Design of Efficient Artificial Enzymes Using Crystallographically Enhanced Conformational Sampling

Behnoush Seifinoferest[1], Rojo V. Rakotoharisoa[2], Niayesh Zarifi[2], Jack D. M. Miller[2], Joshua M. Rodriguez[1], Michael C. Thompson[1], Roberto A. Chica[2]

[1]University of California, Merced, CA, USA. [2]University of Ottawa, Ottawa, Ontario, Canada

11:00 - 11:30am

261 Adaptation of Enzyme Catalysis Across a Natural Evolutionary Landscape

Duncan Muir, Garrison Asper, Jacob Posner, Michael Keiser, Margaux Pinney

University of California, San Francisco, San Francisco, CA, USA

3.1.4 Data Analysis Software & Applications

8:30 - 11:30am Wednesday, 10th July, 2024
Evergreen C
Derek Mendez, Stephen Meisburger

Data analysis techniques in the structural sciences are changing rapidly. State-of-the-art machine learning methods are increasingly used to extract subtle information from large electron and X-ray datasets. Of special note are new techniques for the study of conformationally heterogeneous systems, for instance in single particle cryo-EM and time-resolved X-ray crystallography. In parallel, data analysis increasingly takes advantage of advanced hardware, such as supercomputing resources and GPU-accelerated processing, and these developments will be essential to the next generation electron and X-ray sources with significantly increased data rates. This session explores the latest innovations in data analysis across structural techniques: cryo-EM, cryo-ET, micro-ED, X-ray scattering, and X-ray diffraction. In particular, we highlight challenges and opportunities for data analysis created by modern methods and advanced computing infrastructure, as well as new structural insights these techniques enable.

8:30 - 8:55am

68 **KINNTREX: A Neural Network Unveils Protein Mechanism from Time Resolved X-ray Crystallography**

Marius Schmidt[1], Tek Malla[2], Peter Schwander[2], Gabi Biener[2]

[1]UWM Physics Department, Milwaukee, Wi, USA. [2]UWM Physics Department, Milwaukee, WI, USA

8:55 - 9:15am

100 **Jungfraujoch: Enabling Kilohertz Data Acquisition and Analysis for the Swiss Light Source 2.0**

Filip Leonarski, Meitian Wang

Paul Scherrer Institute, Villigen, Aargau, Switzerland

9:15 - 9:35am

337 **Sensitive Detection of Structural Differences within a Statistical Framework for Comparative Crystallography**

Doeke Hekstra[1], Harrison Wang[1], Margaret Klureza[1], Jack Greisman[1,2], Kevin Dalton[1,3]

[1]Harvard University, Cambridge, MA, USA. [2]DE Shaw Research, New York, NY, USA. [3]New York University, New York, NY, USA

9:35 - 10:00am

122 Benchmarking tools to analyze conformational landscapes with cryo-EM

Laurel Kinman[1], Andrew Grassetti[2], Maria Carreira[1], Joseph Davis[1]

[1]MIT, Cambridge, MA, USA. [2]Aera Therapeutics, Cambridge, MA, USA

10:30 - 10:50am

264 Laue-DIALS: open-source software for polychromatic X-ray diffraction data

Rick Hewitt[1], Kevin Dalton[1], Derek Mendez[2], Harrison Wang[1], Margaret Klureza[3], Dennis Brookner[1], Vukica Šrajer[4], Nicholas Sauter[5], Aaron Brewster[5], Doeke Hekstra[1]

[1]Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, USA. [2]SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [3]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, USA. [4]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL, USA. [5]Molecular Biophysics & Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

10:50 - 11:10am

272 Current and future strategies for end-to-end data analysis at LCLS

Fred Poitevin, Richard Claus, Dan Damiani, Christopher Ford, Mikhail Dubrovin, Wilko Kroeger, Stefano Marchesini, Valerio Mariani, Riccardo Melchiorri, Silke Nelson, Chris O'Grady, Julieth Otero, Omar Quijano, Murali Shankar, Monarin Uervirojnangkoorn, Matthew Weaver, Seshu Yamajala, Cong Wang, Jana Thayer

SLAC National Accelerator Laboratory, Menlo Park, CA, USA

11:10 - 11:30am

348 The UNTANGLE Challenge for revealing cooperative motions

James M Holton

UCSF/LBNL/SLAC, Berkeley, CA, USA

3.1.5 Structural Characterizations Of Emerging Energy Materials

8:30 - 11:30am Wednesday, 10th July, 2024
Evergreen D
Rebecca Smaha, Huiwen Ji

When designing and optimizing next-generation energy materials, careful structural characterizations are crucial for establishing precise structure-property relationships. This session invites works that utilize or develop structural characterization solutions for emerging energy materials in batteries, fuel cells, photovoltaics, thermoelectrics, piezoelectric devices, etc. Possible topics may focus on the steady-state or time-resolved structures of crystalline, disordered, or amorphous materials to correlate with performance or degradation.

8:30 - 8:55am

58 The nature of dynamic local order in hybrid lead halide perovskites

Nicholas Weadock[1], Tyler Sterling[1], Julian Vigil[2,3], Ballal Ahammed[4], Matthew Krogstad[5], Feng Ye[6], David Voneshen[7], Peter Gehring[8], Andrew Rappe[9], Hans-Georg Steinrueck[10], Elif Ertekin[4], Hemamala Karunadasa[3], Dmitry Reznik[1], Michael Toney[1]

[1]University of Colorado Boulder, Boulder, CO, USA. [2]University of California Berkeley, Berkeley, CA, USA. [3]Stanford University, Stanford, CA, USA. [4]University of Illinois Urbana Champaign, Champaign, IL, USA. [5]Argonne National Laboratory, Lemont, IL, USA. [6]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [7]Rutherford Appleton Laboratory, Didcot, Oxfordshire, United Kingdom. [8]National Institute of Standards and Technology, Gaithersburg, MD, USA. [9]University of Pennsylvania, Philadelphia, PA, USA. [10]Forschungszentrum Jülich, Juelick, North Rhine-Westphalia, Germany

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8:55 - 9:20am

21 Hydrogen Storage in Flexible Frameworks

Ryan Klein[1,2], Craig Brown[2], C. Michael McGuirk[3], Arijit Halder[3], Sarah Shulda[1], Philip Parilla[3], Lukas Bingel[4], Krista Walton[4], Dominik Halter[5], Jeffrey Long[5]

[1]National Renewable Energy Laboratory, Golden, CO, USA. [2]NIST Center for Neutron Research, Gaithersburg, MD, USA. [3]Colorado School of Mines, Golden, CO, USA. [4]Georgia Institute of Technology, Atlanta, GA, USA. [5]University of California, Berkeley, Berkeley, CA, USA

9:20 - 9:40am

107 The long and short of it: Combining X-ray Diffraction, PDF, Neutron PDF and EXAFS to elucidate both long-range and short-range defects in Magnesium Cathode Materials

Saul Lapidus, Erik Sarnello

Argonne National Laboratory, Lemont, IL, USA

9:40 - 10:00am

227 Exploring the structural phase space of layered ternary nitride Sc-Ta-N

Baptiste Julien

National Renewable Energy Laboratory, Golden, CO, USA

10:30 - 10:54am

185 Long- and short-range structure in layered battery materials and magnetic materials

Joshua Bocarsly

University of Houston, Houston, TX, USA

10:54 - 11:12am

221 Single crystal diffuse scattering analysis of short-range order in garnet-type Li-ion conductor $Li_{6.75}La_3Nb_{0.25}Zr_{1.75}O_{12}$

Caleb Ramette[1], Zachary Morgan[2], Feng Ye[2], Matthew Krogstad[3], Satya Kushwaha[4,5], Tyrel McQueen[4,5], Huiwen Ji[1]

[1]University of Utah, Salt Lake City, UT, USA. [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [3]Argonne National Laboratory, Lemont, IL, USA. [4]PARADIM Bulk Materials Discovery Facility, Baltimore, MD, USA. [5]Johns Hopkins University, Baltimore, MD, USA

11:12 - 11:30am

231 Compositional effects on the triple conduction behavior of Ba[$Co_xFe_{0.8-x}Zr_{0.1}Y_{0.1}$]$O_{3-\delta}$ (BCFZY) - *Insights from neutron total scattering studies*

Kennedy Agyekum[1], Bernadette Cladek[1], Yewon Shin[2], Jue Liu[3], Ryan O'Hayre[2], Sossina Haile[4], Katharine Page[1,3]

[1]University of Tennessee, Knoxville, Knoxville, Tennessee, USA. [2]Colorado School of Mines, Golden, Colorado, USA. [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [4]Northwestern University, Evanston, Illinois, USA

3.1.6 Developments In Data Collection & Automation In MicroED

8:30 - 11:30am Wednesday, 10th July, 2024
Conifer Ballroom
Brandon Mercado, Shao-Liang Zheng

8:30 - 8:54am

117 Automated serial (rotation) electron diffraction for high-throughput structure determination and phase analysis of complex polycrystalline samples

Paul Hager[1,2], Xiaodong Zou[1,2]

[1]Department of Materials and Environmental Chemistry, Stockholm, Stockholms län, Sweden. [2]Wallenberg Initiative Materials Science for Sustainability, Department of Materials and Environmental Chemistry, Stockholm, Stockholms län, Sweden

8:54 - 9:16am

136 How 3D electron diffraction reveals all about crystal structure

Petr Brazda

Institute of Physics of the Czech Academy of Sciences, Prague 8, N/A, Czech Republic

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9:16 - 9:38am

188 An automated approach to MicroED enables analysis of complex samples

Johan Unge[1,2], Jieye Lin[2], Sara J Weaver[2], Ampon Sae Her[2], Tamir Gonen[2,3,4]

[1]Umea University, Umea, sweden, Sweden. [2]Department of Biological Chemistry, University of California, Los Angeles, Los Angeles, CA, USA. [3]Department of Physiology, University of California, Los Angeles, Los Angeles, CA, USA. [4]Howard Hughes Medical Institute, University of California, Los Angeles, Los Angeles, CA, USA

9:38 - 10:00am

191 Diffraction-Guided Natural Product Discovery

Hosea Nelson

Caltech, Pasadena, Ca, USA

10:30 - 10:50am

109 XtaLAB Synergy-ED and CrysAlis$^{\text{Pro}}$: An update from the software perspective

Mathias Meyer[1], Przemyslaw Stec[1], Michal Jasnowski[1], Grzegorz Prochniak[1], Robert Buecker[2], Oleg Dolomanov[3], Horst Puschmann[3]

[1]Rigaku Polska, Wroclaw, DE, Poland. [2]RESE, Frankfurt, DE, Germany. [3]OlexSys, Durham, DE, United Kingdom

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10:50 - 11:10am

266 Mosaic 3D molecular crystal lattices ironed out by electron beam induced damage

Niko Vlahakis, Arden Clauss, Jose Rodriguez

University of California, Los Angeles, Los Angeles, CA, USA

11:10 - 11:30am

244 4-Dimensional Scanning Transmission Electron Microscopy (4D-STEM): An Emerging Technique for Imaging and Structure Determination

Roger Durst[1], Niels de Jonge[1], Sergey Lazarov[1], Jeorg Kaercher[2]

[1]Bruker AXS, Karlsruhe, BW, Germany. [2]Bruker AXS, Madison, WI, USA

Exhibit Hall

10:00am - 12:00pm Wednesday, 10th July, 2024

PL2: Buerger Award: Thomas Schoenzart

11:45am - 12:45pm Wednesday, 10th July, 2024
Evergreen A
Allen Oliver

M.J. Buerger was a mineralogist who made major contributions to many areas of structural science and this award, in his name, was established to recognize mature scientists who have made contributions of exceptional distinction. In Denver, Colorado we will bestow this award on Thomas Albrecht-Schoenzart. Mr. Albrecht-Schoenzart is a prolific solid-state inorganic chemist who is transforming our understanding of the periodic table through his structural studies of f-block elements. His studies of the structure and bonding in radioactive heavy element compounds have expanded our understanding of the f-block elements and redefined the chemistry of the actinide elements and even the periodic table. We look forward to celebrating Thomas Albrecht-Schoenzart's remarkable achievements and acknowledging the vital role he has played in advancing structural science research.

11:50am - 12:40pm

6 A Race Against Time: Crystallography in the Outer Limits of the Periodic Table

Thomas Albrecht-Schoenzart

Colorado School of Mines, Golden, Colorado, USA

3.3.2 DEI Session: #IAmRemarkable [Pre-registration Required]

12:45 - 1:45pm Wednesday, 10th July, 2024
Evergreen B
Callie Saeher, Sandra Gabelli

Pre-Registration is required for this session and the max capacity will be 20 attendees. Please see the main meeting site for the link to register (www.acameeting24.com).

#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve the self promotion motivation and skills and challenge the social perception around self promotion. Many of us struggle to talk about and celebrate our accomplishments often due to cultural and gender norms. Through our facilitator sessions, #IAmRemarkable helps thousands of people learn the importance of self-promotion in their personal and professional life.

12:45 - 1:45pm

359 #IAmRemarkable

Sandra Gabelli[1], Ampon Saeher[2], Jill Chrencik[1]

[1]Merck, Landsdale, PA, USA. [2]UCLA, Ontario, CA, USA

3.2.1 Flexibility, Dynamics, And The Secret Lives Of Proteins Part 2

2:00 - 5:00pm Wednesday, 10th July, 2024
Evergreen B
Marcus Fischer, Tim Stachowski

Proteins are notorious shapeshifters that change conformations in response to environmental cues like temperature, pH, and ligand binding. This flexibility often underpins biological processes like enzyme catalysis and signal transduction. Recent advances in technologies and modeling algorithms move beyond understanding protein structures as static images and closer to generating molecular movies of proteins throughout their active lifecycles. In turn, these experiments can reveal new opportunities to modulate protein function for therapeutics and biology. This session will focus on emerging methods for exploring protein flexibility, examples where flexibility reveals functional insights, and applications in modulating proteins and drug design.

2:00 - 2:20pm

152 TraG-edy to Triumph: How Challenges in Crystallisation Efforts of TraG Led to Success

Nicholas Bragagnolo, Gerald Audette

York University, Toronto, Ontario, Canada

2:20 - 2:40pm

102 Cryo-EM and Molecular Dynamics Simulations Reveal Hidden Conformational Dynamics Controlling Ammonia Transport in Human Asparagine Synthetase

Yuichiro Takagi[1], Wen Zu[2], Matthijn Vos[3], Vincent Chaptal[4], Nigel Richards[5]

[1]Indiana University School of Medicine, Indianapolis, Indiana, USA. [2]Florida State University, Tallahassee, Florida, USA. [3]Institut Pasteur, Paris, Paris region, France. [4]University of Lyon, Lyon, Auvergne-Rhone_Alpes region, France. [5]Cardiff University, Cardiff, Wales, United Kingdom

2:40 - 3:00pm

40 Exploring the role of Entropy-Enthalpy compensation in protein crystallization with Molecular Dynamics

Nooriel Banayan[1,2], Arthur Palmer[1], John Hunt[1], Elaine Zhang[1], Will Hyatt[1]

[1]Columbia University, New York, NY, USA. [2]SUNY Downstate, NY, NY, USA

3:30 - 4:00pm

81 What can we learn from MD simulations of biomolecular crystals?

David Case

Rutgers University, Piscataway, NJ, USA

4:00 - 4:30pm

93 A Structural Perspective on the Temperature-dependent Activity of Enzymes

Matthew McLeod[1], Sarah Barwell[2], Todd Holyoak[2], Robert Thorne[1]

[1]Cornell, Ithaca, NY, USA. [2]University of Waterloo, Waterloo, ON, Canada

4:30 - 5:00pm

179 How biochemists became flexible in their views on the ability of structural techniques to illuminate the dynamics of proteins

Gregory Petsko

Harvard Medical School, Boston, Massachusetts, USA

3.2.2 Structure of Nucleic Acids - Part 2: SAS/Hybrid Approaches

2:00 - 5:00pm Wednesday, 10th July, 2024
Evergreen A
Michal Hammel, Sarah Keane

This session will highlight the utility of small-angle scattering and in combination with other structural techniques for determining nucleic acid structures and their protein complexes. The session will also highlight success stories where small-angle scattering was used to validate predicted RNA, RNA-protein, or DNA-protein structures. Studies may also include X-ray crystallography, XFEL, CryoEM, or hybrid methods, including those incorporating predictive/computational modeling.

2:00 - 2:30pm

90 Defining and controlling protein allostery and nucleic acid sculpting

John Tainer

Univ. of Texas MD Anderson Cancer Center, Houston, TX, USA

2:30 - 3:00pm

339 Using SAXS, AFM and neural networks to probe RNA conformational space in solution

Maximilia Degenhardt[1], Yun-Tzai Lee[2], Hermann Degenhardt[1], Yun-Xing Wang[1]

[1]NCI, Frederick, MD, USA. [2]NCI, Frederick, md, USA

3:30 - 4:00pm

243 A new view of RNA folding using time-resolved WAXS at XFELs

Lois Pollack

Cornell University, Ithaca, NY, USA

4:00 - 4:15pm

137 Viral RNA structural mimics of the mRNA 5' cap

Deepak Koirala

University of Maryland Baltimore County, Baltimore, MD, USA

4:15 - 4:30pm

115 Solution Scattering (SAXS) for identifying small molecule inhibitors

Greg Hura

Lawrence Berkeley National Lab, Berkeley, CA, USA

4:30 - 4:45pm

98 SAXS/SANS as a structural tool to study RNA:RNA complexes

Aldrex Munsayac[1], Wellington Leite[2], Jesse Hopkins[3], Ian Hall[1], Hugh O'Neill[2], Sarah Keane[1]

[1]University of Michigan, Ann Arbor, MI, USA. [2]Oak Ridge National Lab, Oak Ridge, TN, USA. [3]Argonne National Lab, Lemont, IL, USA

4:45 - 5:00pm

168 Structural basis for apical loop recognition of miR-20a processing by hnRNPA2B1

Sarah Keane

University of Michigan, Ann Arbor, MI, USA

3.2.3 MicroED for Small Molecules

2:00 - 5:00pm Wednesday, 10th July, 2024
Evergreen C
Joseph Ferrara, Christos Malliakas, Anahita Pakzad

MicroED is becoming a mainstream technique for solving structures intractable to conventional X-ray diffraction techniques. Examples of materials that yielded to MicroED include MOFs, natural products and many other materials only available as a powder. In this half-day session, we will explore current trends in micro-electron diffractions and best practices for data collection, processing and refinement.

2:00 - 2:20pm

319 Absolute Structure Determination of a Guanitrypmycin Natural Product by Micro Electron Diffraction

IanDuncan Williams[1], Akihito Yamano[2], Wenkang Ye[1], Peiyuan Qian[1], Herman H-Y. Sung[1]

[1]Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong. [2]Rigaku Corporation, Tokyo, Akishima-shi, Japan

2:20 - 2:40pm

15 Single Crystal Electron and Powder Diffraction of the Anhydrous and Dihydrate Crystalline Forms of a 24-Atom Triazine Macrocycle

Joseph Reibenspies[1], Nattamai Bhuvanesh[1], Mark Del Campo[2], Casey Patterson-Gardner[3], Eric Simanek[3]

[1]Texas A&M University, College Station, Texas, USA. [2]Rigaku Americas Corp., Woodlands, Texas, USA. [3]Texas Christian University, Fort Worth, Texas, USA

2:40 - 3:00pm

53 Structure Determination of Difficult to Grow Active Pharmaceutical Ingredients (APIs) using MicroED

Collin Morris, Rodger Henry, Ahmad Sheikh

AbbVie, North Chicago, IL, USA

3:30 - 4:00pm

42 3D-ED: The potential and the problems with a step change for small-molecule single crystal structure determination

Simon Coles

University of Southampton, Southampton, Hampshire, United Kingdom

4:00 - 4:20pm

254 Sub-Atomic Resolution Imaging of Crystals by Electron Diffraction

Jung Cho[1], Ambarneil Saha[2], Matthew Mecklenburg[1]

[1]California NanoSystems Institute at University of California, Los Angeles, Los Angeles, CA, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

4:20 - 4:35pm

245 Challenges and Victories: Variable Temperature MicroED on Small Molecules

Lee Daniels[1], Khai-Nghi Truong[2], Robert Bücker[2], Christian Göb[2], Christian Schürmann[2], Jakub Wojciechowski[2], Mathias Meyer[3]

[1]Rigaku Americas Corp, The Woodlands, TX, USA. [2]Rigaku Europe SE, Neu-Isenburg, X, Germany. [3]Rigaku Polska, Wrocław, X, Poland

4:35 - 4:50pm

133 MerlinEM, the universal detector for 4D STEM and microED

Gearóid Mangan, Matúš Krajňák

Quantum Detectors Ltd, Harwell, Oxfordshire, United Kingdom

3.2.4 Serial Crystallography

2:00 - 5:00pm Wednesday, 10th July, 2024
Evergreen EF
Daniel Paley, Art Lyubimov

Serial crystallography has emerged as a powerful method for structure determination. At X-ray free electron lasers, "diffraction before destruction" is now a standard technique for studying macromolecules, with unique applications in time-resolved experiments ranging from seconds to femtoseconds. Synchrotron and electron radiation offer new opportunities for growing the availability and scope of serial data collection. The field is also finding applications outside of macromolecular structures, with growing interest in serial diffraction for chemical/small-molecule crystallography. These diverse methods and applications are driving the development of new techniques for sample delivery, instrumentation, and data processing. Especially, the growing data rates in the field (currently in the kHz range at XFEL sources) present an opportunity for applying modern tools in AI and high-performance computing. This session highlights these new advances and the future prospects for serial crystallography as a modern and growing structural technique.

2:00 - 2:20pm

89 Structural changes in Photosystem II using time-resolved X-ray free-electron (XFEL) crystallography and crystalline molecular dynamics.

Asmit Bhowmick[1], Rana Hussein[2], Philipp Simon[1], Jan Kern[1], Vittal Yachandra[1], Junko Yano[1]

[1]LBNL, Berkeley, CA, USA. [2]HU Berlin, Berlin, Berlin, Germany

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2:20 - 2:40pm

129 Time-Resolved Serial Crystallography and Spectroscopy on Earth with the XFEL Hub at Diamond

Allen Orville, Pierre Aller, Anastasya Shilova

Diamond Light Source, Didcot, Oxfordshire, United Kingdom

2:40 - 3:00pm

23 *Sample preparation for routine and advanced structural biology, including serial data collection and microED*

Patrick Shaw Stewart

Douglas Instruments Ltd, Hungerford, Berkshire, United Kingdom. University of Southampton, Southampton, Hampshire, United Kingdom

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3:30 - 4:00pm

128 Determining the Enzymatic Mechanism of DJ-1 Using a New Approach to Mix-and-Inject Synchrotron Serial Crystallography

Kara Zielinski[1], Cole Dolamore[2], Kevin Dalton[3,4], Doeke Hekstra[3,5], Robert Henning[6], Vukica Srajer[6], Mark Wilson[2], Lois Pollack[1]

[1]School of Applied and Engineering Physics, Cornell University, Ithaca, NY, USA. [2]Department of Biochemistry and the Redox Biology Center, University of Nebraska, Lincoln, Lincoln, NE, USA. [3]Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, USA. [4]Department of Biology, New York University, New York, NY, USA. [5]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA. [6]BioCARS, Center for Advanced Radiation Sources, The University of Chicago, Lemont, IL, USA

4:00 - 4:30pm

119 XFEL and Electron Crystallography of Organic Compounds

Koji Yonekura

RIKEN SPring-8, Sayo, Hyogo, Japan. Tohoku University, Sendai, Miyagi, Japan

4:30 - 5:00pm

246 Development of Anaerobic Tools to Determine the Structure of the Active Ni(I) State of Methyl-Coenzyme M Reductase: Nature's Catalyst for Methane Synthesis, Activation, and Oxidation

Christopher Ohmer[1], David Villareal[1], Medhanjali Dasgupta[2], Darya Marchany-Rivera[3], Philip Simon[4], Hiroki Makita[4], Jan Kern[4], Vittal Yachandra[4], Junko Yano[4], Aina Cohen[3], Stephen Ragsdale[1]

[1]University of Michigan, Ann Arbor, MI, USA. [2]University of Nebraska Medical Center, Omaha, NE, USA. [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [4]Lawrence Berkeley National Lab, Berkeley, CA, USA

3.2.5 A Hitchhiker's Guide to Peer Review

2:00 - 5:00pm Wednesday, 10th July, 2024
Evergreen D
Josh Chen, Dan Decato

Peer review is an indispensable part of the scientific publishing world. However, it is often overlooked in STEM programs, leaving many researchers to tackle this crucial process with limited training. As a result, they may lack formal education on how to effectively conduct a review, which can ultimately lead to their assignment as the dreaded "reviewer 2." This session aims to address various aspects of peer review, including how to handle requests, deciding whether to accept or reject manuscripts, providing constructive criticism, understanding the role of editors, distinguishing major and minor considerations, maintaining rational reviews, and effectively dealing with feedback.

2:00 - 2:20pm

145 Rejection without review: "I think you ought to know I'm feeling very depressed."

William Pennington, Colin McMillen

Clemson University, Clemson, SC, USA

2:20 - 2:40pm

224 Peer Review for Beginners and Beyond

Alexander Erickson

Marquette University, Milwaukee, WI, USA

2:40 - 3:00pm

215 A Guide to Reviewing Tables, Graphs, and Figures

Louise Dawe

Wilfrid Laurier University, Waterloo, ON, Canada

3:30 - 3:50pm

257 Don't Panic! Navigating Scientific Peer Review

Sarah Bowman

Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA

3:50 - 4:10pm

265 Almost, but not quite, entirely unlike proteins

Vincent Chen, Christopher Williams, Michael Prisant, David Richardson, Jane Richardson

Duke University, Durham, NC, USA

3.2.6 Alternative Methods For Structure Determination

2:00 - 5:00pm Wednesday, 10th July, 2024
Conifer Ballroom
Jue Liu, Luca Izzolino

This session aims to showcase work involving computational and experimental methods alternative to traditional single-crystal X-ray diffraction for predicting and solving crystal structures of organic small molecules and functional inorganic compounds, with the goal of demonstrating their impact on real-life projects. Examples include but are not limited to, three-dimensional electron diffraction, small angle scattering, crystal structure prediction (CSP) methods, solid-state NMR techniques, structure solution from powder diffraction and total scattering data, and the combination of any of these techniques.

2:00 - 2:30pm

124 Structure determination by NMR Crystallography, from microcrystalline powders to amorphous molecular solids

Lyndon Emsley

EPFL, Lausanne, Vaud, Switzerland

2:30 - 3:00pm

20 Quantitative matching of crystal structures to experimental powder diffractograms

Erin Johnson

Dalhousie University, Halifax, NS, Canada

3:30 - 4:00pm

177 Solving complex structures for Na-ion batteries from powder diffraction

Hao Liu

Binghamton University, Binghamton, NY, USA

4:00 - 4:30pm

143 PtychoSAXS: Combined X-ray ptychography and SAXS imaging for nanostructure characterization

Joseph McCourt, Junjing Deng, Byeongdu Lee, Soenke Seifert

Argonne National Laboratory, Argonne, IL, USA

4:30 - 5:00pm

198 Understanding the structure of $LiNiO_2$

Jue Liu

Oak Ridge National Lab, Oak Ridge, TN, USA

Exhibit Hall

2:00 - 7:30pm Wednesday, 10th July, 2024

PS3: Poster Session #3

5:00 - 7:30pm Wednesday, 10th July, 2024
Atrium

54 Time-Resolved Macromolecular Crystallography Frontiers at BioCARS: Serial Laue Micro-Crystallography and Electric Field Jump

Robert Henning[1,2], Vukica Srajer[1,2], Irina Kosheleva[1,2], Insik Kim[1,2], Eric Zoellner[1,2], Rama Ranganathan[1,2]

[1]University of Chicago, Chicago, IL, USA. [2]Sector 14 BioCARS, APS Argonne National Laboratory, Lemont, IL, USA

370 Current capabilities and new initiatives of the Advanced Crystallographic Program at NSF's ChemMatCARS

Jinxing Jiang[1], Tieyan Chang[2], Kevin Lynch[2], Yu-Sheng Chen[2]

[1]The University of Illinois Chicago, Chicago, Illinois, USA. [2]The University of Chicago, Chicago, Illinois, USA

393 The Structure of Apo *Acinetobacter baumannii* Dithiol Oxidase DsbA and Isothermal Titration Calorimetry Validation of DsbA for Antimicrobial Drug Development

Kyung Hyeon Lee[1,2], Soo Hyeon Lee[2], Iswarduth Soojhawona[2], Misgina Girma[1], Kayla Davis[2], Nagarajan Pattabiraman[3], Schroeder Noble[2]

[1]George Mason University, Manassas, VA, USA. [2]Walter Reed Army Institute of Research, Silver Spring, MD, USA. [3]MolBox LLC, Silver Spring, MD, USA

394 Using Hydrodynamics, Crowders and Kosmotropes to turn a $k_{can't}$ into a k_{cat}

Zachary Wood, Jeong-Yeh Yang, Renuka Kadirvelraj, Justin Sanders, Kelley Moremen

University of Georgia, Athens, GA, USA

43 Raw Data Letters - describing and publishing raw diffraction data in a FAIR way

Simon Coles[1], Loes Kroon-Batenburg[2], John Helliwell[3], James Hester[4]

[1]University of Southampton, Southampton, Hampshire, United Kingdom. [2]Utrecht University, Utrecht, Utrecht, Netherlands. [3]University of Manchester, Manchester, Greater Manchester, United Kingdom. [4]ANSTO, Lucas Heights, New South Wales, Australia

66 Achieving high-throughput, high-quality imaging for SPA with HexAuFoil® sample supports

Claire Naylor[1], Paul Thaw[2], Herve Vandekerckhove[2]

[1]Quantifoil Micro Tools GmbH, Jena, Thuringia, Germany. [2]SPT Labtech, Melbourn, Cambridge, United Kingdom

345 Development of SPring-8 BL41XU toward time resolved serial crystallography

Kazuya Hasegawa[1], Naomine Yano[1], Hideo Okumura[1], Seiki Baba[1], Takashi Kawamura[1], Hironori Murakami[1], Takuya Masunaga[1], Nipawan Nuemket[1,2], Jungmin Kang[2], Toshiaki Hosaka[3], Masaki Yamamoto[2], Eriko Nango[4], Takashi Kumasaka[1]

[1]Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan. [2]RIKEN SPring-8 Center, Sayo, Hyogo, Japan. [3]RIKEN Center for Biosystems Dynamics Research, Yokohama, Kanagawa, Japan. [4]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi, Japan

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351 Minimising the payload solvent exposed hydrophobic surface area optimises the antibody-drug conjugate properties

Adrian Hobson[1], Haizhong Zhu[2], Wei Qiu[2], Russell Judge[2], Kenton Longenecker[2]

[1]Abbvie Bioresearch Center, Worcester, MA, USA. [2]Abbvie Inc, North Chicago, IL, USA

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362 Metabolic Enzymes Moonlighting as RNA Binding Proteins

Nicole Curtis[1], Geordie Emberling[2], Alquama Lokhandwala[2], Mary Jo Ondrechen[2], Constance Jeffery[1,2]

[1]University of Illinois at Chicago, Chicago, IL, USA. [2]Northeastern University, Boston, MA, USA

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378 Leveraging Advances in Cryo Electron Microscopy to Facilitate Drug Discovery

Nicole Poweleit, Claudio Catalano, Kyle Lucier, Skerdi Senko, Nhi Tran, Ashlyn Farwell, Giovanna Scapin

NanoImaging Services, San Diego, CA, USA

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381 Rare conformations in RNA backbone

Christopher Williams, Jane Richardson

Duke University, Durham, NC, USA

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390 Exploring Validation of PDB Experimental Structures and Computed Structure Models at RCSB.org

Maria Voigt, Stephen Burley

RCSB Protein Data Bank, Piscataway, NJ, USA

404 Equilibrium and Time-Resolved SAXS at BioCAT

Maxwell Watkins, Jesse Hopkins, Mark Vukonich, Richard Heurich, Carrie Clark, Thomas Irving

Illinois Institute of Technology, Lemont, Illinois, USA

37 Using X-ray footprinting mass spectrometry to investigate structural changes of proteins in solution

Sayan Gupta[1], Line Kristensen[1], Sathi Paul[1], Simruthi Subramanian[1], Savannah Kidd[1], Darran Kahan[2], Jamie Inman[1], Antoine Snijders[1], Corie Ralston[1]

[1]Lawrence Berkeley National Lab, Berkeley, CA, USA. [2]University of California, Berkeley, CA, USA

222 Judging Data Quality in Reciprocal Space

Ashley Weiland Schmidt

Bruker, Madison, WI, USA

286 Smarter targeting for screening and data collection in Leginon

William Rice, Bing Wang, Huihui Kuang

NYU Langone Health, New York, NY, USA

357 The Open Plunge Initiative: a modular and quality assessment platform for vitrification technology evaluation

Albert Konijnenberg[1], Bas Hendriksen[1], Jolet de Ruiter[1], Leander de Boer[1], Pleun Dona[1], Christian Lamberz[1], Xue Wang[1], Natalya Dudkina[1], Aurelien Botman[2], Edward Pryor[2]

[1]Thermo Fisher, Eindhoven, Noord-Brabant, Netherlands. [2]Thermo Fisher, Hillsboro, Oregon, USA

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360 Structure-based chemical probe development of the PWWP domain containing proteins

Jinrong Min

University of Toronto, Toronto, Ontario, Canada. Central China Normal University, Wuhan, Hubei, China

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373 PADT: A novel GUI for serial data classification using Machine Learning approaches

Sabine Botha, Gihan Ketawala

Arizona State University, Tempe, AZ, USA

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416 *Plasmodium falciparum* Bromodomain Protein 1 (PfBDP1): A master regulator of red blood cell invasion genes

Karen Glass[1], Ajit Singh[1], Mirabella Vulikh[1], Margaret Phillips[1], Marco Tonelli[2], Trushar Patel[3], Borries Demeler[3], Jay Nix[4]

[1]University of Vermont, Burlington, VT, USA. [2]University of Wisconsin, Madison, WI, USA. [3]University of Lethbridge, Lethbridge, AB, Canada. [4]Advanced Light Source, Berkeley, CA, USA

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419 Mix-and-Quench Technology for Efficient and Routine Time-Resolved Crystallography

John Indergaard[1], Matthew McLeod[1], Kashfia Mahmood[2], Leo Gabriel[2], Gary Zhong[2], Robert Thorne[1]

[1]Cornell University, Ithaca, NY, USA. [2]University of Waterloo, Waterloo, Ontario, Canada

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318 Structural insight into polymerase mechanism via a chiral center generated with a single selenium atom

Tong Qin[1], Bei Hu[2], Yiqing Chen[3], Jianhua Gan[4], Zhen Huang[1,5]

[1]College of Life Sciences, Sichuan University, Chengdu, Sichuan, China. [2]College of Life Sciences, Sichuan UniversityZh, Chengdu, Sichuan, China. [3]School of Life Sciences, Fudan UniversityChen, Shanghai, Shanghai, China. [4]School of Life Sciences, Fudan University, Shanghai, Shanghai, China. [5]SeNA Research Institute, Chengdu, Sichuan, China

27 Engaging Students with Small-Molecule Crystallography: Strategies for Effective Education and Research Integration

Shao-Liang Zheng

Harvard University, Cambridge, MA, USA

377 Striving to Meet the Needs of the Structural Biology Community at the National Crystallization Center

Gabrielle Budziszewski[1], Tiffany Wright[1], M. Elizabeth Snell[1], Miranda Lynch[1], Sarah E. J. Bowman[1,2]

[1]Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA. [2]University at Buffalo, Buffalo, NY, USA

385 Tunable Energy Synchrotron Diffraction Anomalous Fine Structure (DAFS) Reveals Unprecedented Insights into Copper Compounds

Tieyan Chang[1], Yu-Sheng Chen[1], Pinar Alayoglu[2], Connly Yan[2], Neal Mankad[2]

[1]The Unversity of Chicago, Lemont, IL, USA. [2]University of Illinois at Chicago, Chicago, IL, USA

411 A Light Source Role: Engaging students in crystallography and beyond

Vivian Stojanof, Aleida Perez

Brookhaven National Laboratory, Upton, NY, USA

422 Development of Methods for the Stabilization of Cryo-EM samples

Mahitha Roy, Dominika Borek, Zbyszek Otwinowski

Univeristy of Texas Southwestern Medical Center, Dallas, TX, USA

423 High Resolution Crystal Structure of SARS-CoV-2 Nucleocapsid Protein N-Terminal Domain with Part of Flexible N-Arm in complex with ssDNA.

Atanu Maiti, Hiroshi Matsuo

Cancer Innovation Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MD, USA

428 A Crystallographic Search for Isomorphism among “Bridge-Flipped” 2,2’-Disubstituted Benzylideneanilines

William Ojala

University of St. Thomas, St. Paul, Minnesota, USA

424 The Berkeley Center for Structural Biology at the Advanced Light Source

Marc Allaire[1], Jeff Dickert[1], John Taylor[1], Kevin Royal[1], Anthony Rozales[1], Stacey Ortega[1], Gabriel Gazolla[1], Kat McLaren[1], Adrian Spucces[1], Antoine Wojdyla[1], Yang Ha[1], Daniil Prigozhin[1], Jay Nix[2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [2]Molecular Biology Consortium, Berkeley, CA, USA

429 BioSAXS measurement and analysis system in Japanese synchrotron radiation facilities, Photon Factory and SPring-8

Nobutaka Shimizu[1,2], Satoshi Nagao[3], Hiroshi Sekiguchi[3,1], Hideaki Takagi[2], Hiroyasu Masunaga[3,1], Masatoshi Maeki[4,1,2], Masaki Yamamoto[1]

[1]RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan. [2]High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan. [3]Japan Synchrotron Radiation Research Institute, Sayo-gun, Hyogo, Japan. [4]Hokkaido University, Sapporo, Hokkaido, Japan

433 Validating cryoEM reconstruction using complex-valued particle stack

Raquel Bromberg[1], Dominika Borek[2], Yirui Guo[1], Zbyszek Otwinowski[2]

[1]Ligo Analytics, Dallas, TX, USA. [2]UT Southwestern Medical Center, Dallas, TX, USA

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434 Deep Learning Insights on Na^+/I^- Symporter (NIS) transport cycle.

Alfonso Leyva[1], Paola Bisignano,[2], Silvia Ravera[3], Alejandro Llorente[2], Eric Aguilar[4], Laura Lopez Rovira[4], Nancy Carrasco[2], Mario Bianchet[4]

[1]Department of Physics Pontificia Universidad Javeriana, Bogota, DC, Colombia. [2]Vanderbilt University, Nashville, TN, USA. [3]Vanderbilt Vaccine Center, Nashville, TN, USA. [4]Johns Hopkins School of Medicine, Baltimore, MD, USA

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438 Observing DNA Polymerase Double Strand Break Synthesis

JOONAS JAMSEN

University of Arkansas for Medical Sciences, Little Rock, AR, USA

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439 3-D Visualization of Crystal Structures Using the CrystalVR Plug-in for ORION

Nichole R. Valdez, Mark A. Rodriguez, Anthony W Alberti, Shane M Bramley, Matt Gallegos, Eric M Nagel, Erica M Redline, Chris DiAntonio

Sandia National Laboratories, Albuquerque, NM, USA

3.3.1 Would You Publish This?

7:30 - 9:30pm Wednesday, 10th July, 2024
Evergreen A
Matthew Brown, Scott Lee

Is your structure too poor to publish? What compromises would you have to make to publish your "low quality" structure? Do you have some less then ideal powder data that you still think you can make something useful with? If you have ever asked yourself these questions, then share your problems, insights, structures, and advice with the crystallography community. This is a great opportunity for young crystallographers to share their work, where they can interact with a friendly audience, who with years of experience will provide constructive advice. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density, suspicious of an incommensurate structure, etc. Talks in this session will be restricted to approximately 5 minutes in order to encourage audience participation and discussion. All talks will be selected from submitted abstracts. Those who submit abstracts to this session may still submit a second abstract to other sessions at no additional fee. This session is open to non-small molecule talks; Powder, protein and other types of crystallography are welcome!

7:30 - 7:35pm

9 Porous Coordination Cages: Acceptable levels of structure completion.

Glenn Yap[1], Michael Dworzak[1], Eric Block[2]

[1]University of Delaware, Newark, DE, USA. [2]Indiana University, Bloomington, IN, USA

7:35 - 7:45pm

95 Is this publishable (please)? Quality in Crystallography

Joseph Reibenspies

Texas A&M University, College Station, Texas, USA

7:45 - 7:55pm

153 How WYPT Aided in the Structure Solution of P1 from *Pseudomonas aeruginosa*

Nicholas Bragagnolo, Gerald Audette

York University, Toronto, Ontario, Canada

7:55 - 8:05pm

154 Poorly Diffracting Samples: What is Weak Data and What is Noise?

Toby Woods

University of Illinois at Urbana-Champaign, Urbana, IL, USA

8:05 - 8:15pm

208 Crystallographic Errors in Published Structures

Diane Dickie

University of Virginia, Charlottesville, VA, USA

8:15 - 8:25pm

268 From the molecular structure of type II collagen to a profound change in student success practice in Chicago (and my own learning disabilities journey)

Joseph Orgel, Rama Madhurapantula

Illinois Tech, Chicago, IL, USA

8:25 - 8:35pm

340 Sufficient chemical answer vs correct handling of a modulated structure

Ilia Guzei[1], Michael Ruf[2], Seth Young[1], Andrew Buller[1]

[1]University of Wisconsin-Madison, Madison, WI, USA. [2]Bruker, Madison, WI, USA

8:35 - 8:45pm

132 Complex Crystallography in Modulated $BiIr_4Se_8$

Scott Lee, Connor Pollak, Grigorii Skorupskii, Leslie Schoop

Princeton University, Princeton, NJ, USA

Registration Desk

7:00 - 11:00am Thursday, 11th July, 2024
Rocky Foyer - Pint Brothers BY

4.1.1 Biological Structures from Artificial Intelligence

8:30 - 11:30am Thursday, 11th July, 2024
Evergreen A
Jeney Wierman, Aaron Brewster

Over the last four years the field of structural biology, for proteins in particular, has experienced a profound change. At synchrotron facilities data is acquired at a breath-taking speed, leaving many a scientist struggling to keep pace with data handling and analysis. The data resolution achieved with cryo-EM has now safely moved into a range that makes atomic model building routine and cryo-imaging as a whole now enables the study of large, macromolecular machines in situ. Lastly, the unprecedented quality of protein models from structure prediction has opened new ways of conducting research in structural biology. Both the prediction of structures and the interpretation of large amounts of high-resolution data, require sophisticated computational models. Hence, machine learning (ML) and artificial intelligence (AI) are now close to becoming standard tools for structural biologists to conduct their data analysis and interpretation. In this session we will look at the most recent ML and AI tools and developments that could now be in any structural biologists data analysis repertoire.

8:30 - 9:00am

83 Quantum-based atomic model refinement becomes reality

Pavel Afonine[1], Malgorzata Biczysko[2], Hatice Gökcan[3], Olexandr Isayev[3], Holger Kruse[4], Nigel Moriarty[1], Mark Waller[4], Roman Zubatyuk[3], Adrian Roitberg[5]

[1]LBNL, Berkeley, CA, USA. [2]SHU, Shanghai, Baoshan, China. [3]CMU, Pittsburgh, PA, USA. [4]Pending AI, Sydney, NSW, Australia. [5]UFL, Gainesville, FL, USA

9:00 - 9:30am

118 Developing Novel Ligands with Binding Affinity Using Machine Learning

Yang Ha

Lawrence Berkeley National Lab, Berkeley, CA, USA

9:30 - 10:00am

205 SFCalculator: enabling crystallographic structure refinement with deep generative models

MINHUAN LI[1], Kevin Dalton[1,2], Doeke Hekstra[1]

[1]Harvard University, Cambridge, MA, USA. [2]New York University, New York, NY, USA

10:30 - 11:00am

104 Predicting protein structure and dynamics with deep learning and solution scattering

Scott Classen, Michal Hammel

LBNL, Berkeley, CA, USA

11:00 - 11:30am

338 AI in Structural BiologyThe Good, The Bad, and The Ugly

Wladek Minor

University of Virginia, Charlottesville, VA, USA

4.1.2 Totally Total Scattering

8:30 - 11:30am Thursday, 11th July, 2024
Evergreen B
Daniel Olds, Benjamin Frandsen

By utilizing both the Bragg and diffuse scattering, total scattering methods, such as pair distribution function (PDF) analysis, probe both the local and long range features of a material. This session will highlight recent applications and method developments in both neutron and x-ray total scattering. Topics encouraged to apply include studies of complex and disordered materials, functional materials, in situ and operando studies, and methods developments from instrumentation to analysis software. As this discipline continues to grow in impact across diverse fields, this session will be useful for newcomers and experienced practitioners alike.

8:30 - 8:48am

196 Probing the li percolation network and the effects of distortion in cation-disordered rock-salt cathode materials

Yuanpeng Zhang

ORNL, Oak Ridge, TN, USA

8:48 - 9:06am

210 Crystallization dynamics of thin film ternary nitrides

Rebecca Smaha

National Renewable Energy Laboratory, Golden, CO, USA

9:06 - 9:24am

147 Local magnetic correlations in ferrimagnetic semiconductor $Mn_3Si_2Te_6$

Raju Baral, Andrew May, Stuart Calder

Oak Ridge National Lab, Oak Ridge, TN, USA

9:24 - 9:42am

280 Impact of thermal annealing on magnetic properties in nano compositionally complex spinel cobaltite - $(Mg_{0.2}Mn_{0.2}Fe_{0.2}Cu_{0.2}Zn_{0.2})Co_2O_4$

Xin Wang[1], Cameron Jorgensen[1], Corisa Kons[1], Yuanpeng Zhang[2], Jue Liu[2], Peter Metz[1], Eleonora Calì[3], Dustin Gilbert[1], Katharine Page[1,2]

[1]University of Tennessee, Knoxville, Knoxville, TN, USA. [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [3]Politecnico di Torino, Turin, Turin, Italy

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9:42 - 10:00am

85 Total X-ray Diffraction (PDF) and Micro-ED as a solution for novel cathode material characterization

Simon Bates, Joseph Ferrara, Pierre LeMagueres, Lee Daniels, Meredith Shi

Rigaku Americas, The Woodlands, Texas, USA

10:30 - 10:50am

167 Characterization of Disordered Nuclear Materials with Neutron Total Scattering Experiments

Eric O'Quinn

University of Tennessee, Knoxville, TN, USA

10:50 - 11:10am

176 Short-range order revealed by 3D-ΔPDF in a Li superionic conductor

Huiwen Ji[1], Caleb Ramette[1], Matthew Krogstad[2]

[1]University of Utah, Salt Lake City, UT, USA. [2]Argonne National Laboratory, Lemont, IL, USA

11:10 - 11:30am

148 Total scattering and the structural instability in the sub-stoichiometric niobium oxide, $NbO_{2-\delta}$

Jared Allred[1], Top Rawot Chhetri[1], Jacob Phillips[1], Matthew Krogstad[2], Jose Sanchez-Rodriguez[1], Arun Gupta[1]

[1]The University of Alabama, Tuscaloosa, AL, USA. [2]Argonne National Laboratory, Lemont, IL, USA

4.1.3 Macromolecular Microcrystal Electron Diffraction

8:30 - 11:30am Thursday, 11th July, 2024
Evergreen C
Dominika Borek, Michael Martynowcyz

Building on the interplay between cutting-edge electron microscopy and minuscule crystal sizes, Macromolecular Microcrystal Electron Diffraction (MicroED) has become an indispensable tool for high-resolution structure determination of biological macromolecules. This session delves into unveiling newly determined macromolecular structures facilitated by MicroED, and exploring the latest innovations and improvements in MicroED methodologies. Attendees will gain insights into the capabilities and future directions of MicroED in solving complex biological structures, from advances in data collection and processing to tackling previously intractable problems in structural biology.

8:30 - 9:00am

28 HeXI: The High-energy Electron Xtallography Instrument at Diamond Light Source

alistair siebert[1], Pedro Nunes[1], Gwyndaf Evans[1,2]

[1]Diamond Light Source, Harwell, Oxfordshire, United Kingdom. [2]Rosalind Franklin Institute, Harwell, Oxfordshire, United Kingdom

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9:00 - 9:30am

300 Electron-counting for MicroED

Johan Hattne[1,2], Michael Martynowycz[2], Max Clabbers[1,2], Tamir Gonen[1,2]

[1]Howard Hughes Medical Institute, Los Angeles, CA, USA. [2]University of California, Los Angeles, Los Angeles, CA, USA

9:30 - 10:00am

160 DNA structure by MicroED

Brent Nannenga

Arizona State University, Tempe, AZ, USA

10:30 - 11:00am

63 Improved targetting for pFIB milling and high-throughput microED data acquisition and processing.

William Nicolas[1], Anna Shiriaeva[2], Michael Martynowycz[3], Tamir Gonen[1]

[1]HHMI, Los Angeles, CA, USA. [2]UCLA, Los Angele, CA, USA. [3]UCLA, Los Angeles, CA, USA

11:00 - 11:30am

84 Macromolecular cryo-crystallography on the XtaLAB Synergy-ED

Pierre Le Magueres[1], Mark Del Campo[1], Joseph Ferrara[1], Jakub Wojciechowski[2]

[1]Rigaku Americas Corporation, The Woodlands, TX, USA. [2]Rigaku Europe SE, Neu-Isenburg, Hesse, Germany

4.1.4 Structural Biology of Metallobiomolecules

8:30 - 11:30am Thursday, 11th July, 2024
Evergreen D
Darya Marchany-Rivera, Sarah Bowman

Metals play critical roles in biology, conferring unique reactivity, enabling challenging chemistry and redox reactions, and functioning as structural scaffolds. It has been estimated that 30-50% of all proteins bind a metal or metal cofactor. Metals present both opportunities and challenges in structure determination. In this session, we will explore the range of structural techniques used to interrogate metallobiomolecules, including diffraction-based, CryoEM, and computational methods.

8:30 - 8:50am

45 A Trp to a Cu binding site

Yuri Rafael Oliveira Silva, Dia Zheng, Oriana Fisher

Lehigh University, Bethlehem, PA, USA

8:50 - 9:10am

232 Structural and Dynamic Regulation of Reactive Intermediates in Cytochrome P450s

Alec Follmer[1], Jessica Gable[1], Vidhi Murarka[1], Ryan Ribson[2], Thomas Kroll[2], Leland Gee[2], Thomas Poulos[1]

[1]UC Irvine, Irvine, CA, USA. [2]SLAC National Accelerator Laboratory, Menlo Park, CA, USA

9:10 - 9:30am

284 Metalloproteins in emerging pathogens

Diana Monteiro[1], Gabby Budziszewski[2], Elizabeth Snell[2], Sarah Bowman[2]

[1]National Cancer Institute, Frederick, MD, USA. [2]Hauptman-Woodward Med. Res. Institute, Buffalo, NY, USA

9:30 - 9:55am

335 New Opportunities to Study Metalloprotein Structure and Dynamics

Aina Cohen

Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Center, Stanford University, Menlo Park, CA, USA

10:30 - 10:45am

5 Novel insights into the mechanism of long-range radical transfer in class Ia ribonucleotide reductase by cryogenic-electron microscopy

Dana Westmoreland[1], Patricia Feliciano[1], Catherine Drennan[1,2]

[1]Massachusetts Institute of Technology, Cambridge, MA, USA. [2]Howard Hughes Medical Institute, Chevy Chase, MD, USA

10:45 - 11:00am

130 Light atoms identification and location by anomalous scattering

Kamel El Omari, Ramona Duman, Christian Orr, Vitaliy Mykhaylyk, Armin Wagner

Diamond Light Source, Didcot, Oxfordshire, United Kingdom

11:00 - 11:15am

195 Intermediate states of nucleotide addition by HIV-1 Reverse Transcriptase

Sandra Vergara, Xiaohong Zhou, Ulises Santiago, James Conway, Nicolas Sluis-Cremer, Guillermo Calero

University of Pittsburgh, Pittsburgh, PA, USA

11:15 - 11:30am

87 Ineffectiveness of D-captopril as an Inhibitor Against VIM-31 Metallo-β-lactamase Due to a Single Mutation Near Its Active Site

Surendra Silwal

Miami University, Oxford, Ohio, USA

4.1.5 Latest Developments, Applications & Experiences Featuring Quantum Crystallography

8:30 - 11:30am Thursday, 11th July, 2024
Evergreen EF
Brian Patrick, Michael Bodensteiner

This session invites all scientists, from practitioners to method developers. In particular, end-users of any kind of quantum crystallographic technique are most welcome to share their experiences and results. Topics may include all theoretical and practical aspects of the application of quantum mechanics to the study of crystalline materials. Presenters are encouraged to show how these methods enable or improve agreement with experimental data to gain a deeper understanding of the material under study. Research areas may range from inorganic solids and networks, to organic and organometallic compounds, to large structures such as proteins.

8:30 - 9:00am

62 Systematic Benchmark of Levels of Theory in NoSpherA2-HAR

Florian Kleemiss, Daniel Bruex

RWTH Aachen University, Aachen, Northrhine-Westphalia, Germany

9:00 - 9:30am

121 Predicting electrostatic and optoelectronic properties of biomolecules via group polarizability approach

Anna Krawczuk, Raphael Fernandes Ligorio

University of Goettingen, Goettingen, Lower Saxony, Germany

9:30 - 10:00am

22 Olex2.refine

Oleg Dolomanov, Horst Puschmann

OlexSys Ltd, Durham, Durham, United Kingdom

10:30 - 11:00am

8 NoSpherA2 in the Hands of a Synthetic Chemist: The Future is Now

René Boeré

University of Lethbridge, Lethbridge, Alberta, Canada

11:00 - 11:30am

64 Quantum Crystallography combined with Neutron Study: Molecular Insights of Crystal Engineering for Carbon Capture Materials

Sylwia Pawledzio[1], Jeffrey Einkauf[2], Radu Custelcean[2], Xiaoping Wang[1]

[1]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

4.1.6 Advances in SAS Instrumentation

8:30 - 11:30am Thursday, 11th July, 2024
Conifer Ballroom
Shuo Qian, Jan Ilavsky

Recent and upcoming facility upgrades of many synchrotron and neutron sources, as well as recent advancements of high-brightness home X-ray sources, provide great opportunities for advances in small-angle scattering instruments for a wide range of applications. For example, the most revolutionary changes - dramatic increase in coherence and brightness - will be offered by the new 4th generation synchrotron sources (APS-U). And at Spallation Neutron Source, the proton power upgrade and the Second Target Station will provide unprecedentedly powerful neutron sources. In this session, we will highlight the new developments and capabilities of SAS instrumentation from both large facilities and home sources, including but not limited to hardware, software, and sample environments.

8:30 - 8:48am

201 Dueling Robots: Concurrent, Robotic, AI-Driven SAXS and SANS to Solve Industrial Problems

Peter Beaucage, Duncan Sutherland, Tyler Martin

National Institute of Standards and Technology, Gaithersburg, MD, USA

8:48 - 9:06am

213 New opportunities for Bonse-Hart Ultra-Small Angle X-ray Scattering enabled by 4th generation APS-U

Jan Ilavsky

Argonne National Laboratory, Lemont, IL, USA

9:06 - 9:24am

19 Designing CENTAUR, the SANS/WANS Diffractometer with high flux and inelastic scattering suppression capabilities at the Second Target Station of SNS

Shuo Qian

Oak Ridge National Laboratory, Oak Ridge, TN, USA

9:24 - 9:42am

314 State of the Art Instruments for Dynamics and Structure: APS-U Feature Beamlines 9-ID and 8-ID

Joseph Strzalka, Zhang Jiang, Jin Wang, Qingteng Zhang, Eric Dufresne, Suresh Narayanan

Argonne National Laboratory, Lemont, IL, USA

9:42 - 10:00am

214 The new USAXS facility at APS-U and its role in carbon dioxide reduction through both ex-situ and in-situ operando capabilities

Andrew Allen

National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA

10:30 - 10:48am

236 New SAXS capabilities at BioCAT after the APS upgrade

Jesse Hopkins[1], Maxwell Watkins[2], Thomas Irving[1]

[1]Illinois Institute of Technology, Chicago, IL, USA. [2]Illinois Institute of Technology, Chicago, Il, USA

10:48 - 11:06am

322 Instrumentation for Biological SAXS at SSRL BL4-2

Thomas Weiss

Stanford University / SSRL, Menlo Park, CA, USA

11:06 - 11:24am

274 Developments at Bio-SANS instrument enables enhanced structural analysis of biological systems and biomaterials

Wellington Leite, Sai Venkatesh Pingali, Felicia Gilliland, Yingrui Shang, Kevin Weiss, Qiu Zhang, Honghai Zhang, Volker Urban, Hugh O'Neill

Oak Ridge National Laboratory, Oak Ridge, TN, USA

PL3: Warren Award: John Greeden

11:45am - 12:45pm Thursday, 11th July, 2024
Evergreen A
Allen Oliver

The Bertram Eugene Warren Diffraction Physics Award is awarded to outstanding scientists to recognize important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. This year we will celebrate John Greedan with this prestigious award at the 74th annual American Crystallographic Association meeting in Denver, Colorado. Mr. Greedan has made tremendous contributions to the research on structure-property relationships in perovskites and pyrochlores. In particular, his body of work on pyrochlores has had an immense impact on the field, making him one of the most influential researchers in this area. He has used neutron diffraction elegantly for both crystal structure and magnetic structure determination. His papers "Magnetic Pyrochlore Oxides" (Rev. Modern Phys. 2010, 82, 53) and "Geometrically frustrated magnetic materials" (J. Mater. Chem. 2001, 11, 37) are highly revered in the field and have been cited thousands of times. Join us in congratulating John Greedan on this well-deserved achievement, in Denver in July of 2024, as we celebrate his remarkable accomplishments in the realm of diffraction physics.

11:50am - 12:40pm

25 Exploring the Structure/Property Nexus in Perovskite and Pyrochlore Oxides

John Greedan

McMaster University, Hamilton, ON, Canada

4.2.1 AI in Modern Crystallography

2:00 - 5:00pm Thursday, 11th July, 2024
Evergreen A
Daniel Olds, Alicia Manjon Sanz

The rapid advancements in artificial intelligence (AI) and machine learning (ML) are revolutionizing various scientific domains, including materials science, chemistry, physics, biology, and others. These methods have found particularly applicability in fields where the data generation rate has outpaced conventional analysis methods, often resulting in a big data bottleneck. This session aims to explore the diverse applications of AI and ML techniques as they are being utilized in crystallography including structure determination, materials characterization, experiment control, facility operation, and data analysis.

2:00 - 2:30pm

35 Integrated AI/ML and HPC Framework for Multidimensional Neutron Crystallography

Xiaoping Wang[1], Guannan Zhang[2], Junqi Yin[3], Siyan Liu[4], Viktor Reshniak[2], Zachary Morgan[1], Sylwia Pawledzio[1], Thomas Proffen[1], Huibo Cao[1], Bryan Chakoumakos[1], Christina Hoffmann[1], Yaohua Liu[5]

[1]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [2]Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [3]National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [4]Computational Science and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [5]Second Target Station, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

2:30 - 3:00pm

52 Distinguishing isotropic and anisotropic signals for X-ray scattering data using machine learning

Danielle Alverson[1], Daniel Olds[2], Megan Butala[1]

[1]University of Florida, Gainesville, FL, USA. [2]Brookhaven National Laboratory, Upton, NY, USA

3:30 - 4:00pm

138 Combined Machine Learning and Exhaustive Symmetry Approach for Phase Transition Studies

Dayton Kizzire, Maksim Eremenko, Matt Tucker, Yuanpeng Zhang

Oak Ridge National Laboratory, Oak Ridge, TN, USA

4:00 - 4:30pm

329 The future of advanced automation at the NSLS-II AMX beamline

Jean Jakoncic

NSLS-II/BNL, Upton, NY, USA

4.2.2 Cool Structures

2:00 - 5:00pm Thursday, 11th July, 2024
Evergreen B
Alexis Davidson, Kamran Ghiassi

This session aims to highlight exciting structures in the realm of chemical crystallography. Examples of 'cool' structures would include small molecules of interest for their chemical or crystallographic properties, structure-property relationships, extended structures, supramolecular materials, and co-crystals. The session will bring the science enabled by chemical crystallographic analysis to the foreground. Speakers will be selected from contributed abstracts. Submissions from students are encouraged.

2:00 - 2:20pm

33 Oxos, Diamond Cores, and Oxides: A Look at Co-O

Sophie Anferov, Joseph Schneider, Alexander Filatov, John Anderson

University of Chicago, Chicago, Illinois, USA

2:20 - 2:40pm

34 Electrostatically Enhanced 3- and 4-Pyridyl Borate Salt Nucleophiles and Bases

Alex Lovstedt, Stephen Dempsey, Steven Kass

University of Minnesota, Minneapolis, MN, USA

2:40 - 3:00pm

248 Polymorphs in a Pandemic: Structure Elucidation of Polymorphs of Molnupiravir

Justin Newman, Andrew Brunskill, Luca Iuzzolino, Jameson Bothe, Melissa Tan

Merck and Co. Inc., Rahway, NJ, USA

3:30 - 3:50pm

103 From 1D to 0D Hybrid Manganese Chloride Structures

Raúl Castañeda, Michael Ozide

New Mexico Highlands University, Las Vegas, NM, USA

3:50 - 4:10pm

242 Biophysical Characterization of the *Pseudomonas aeruginosa* BqsR/BqsS Two-Component System

Alexander Paredes[1], Chioma Iheacho[1], Darryn Greene[1], Kelly Chacón[2], Aaron T. Smith[1]

[1]University of Maryland Baltimore County, Baltimore, MD, USA. [2]Reed College, Portland, Oregon, USA

4:10 - 4:30pm

79 Characterization and structural determination of self-assembling noncanonical cyclized peptides

Jessalyn Miller[1], Vincent Conticello[2], Andres Gonzalez Socorro[2], Jerry Wang[3], Javier Montenegro García[4]

[1]New York Structural Biology Center, New York, NY, USA. [2]Emory University, Atlanta, GA, USA. [3]The University of Alabama at Birmingham, Birmingham, AL, USA. [4]Universidade de Santiago de Compostela, Santiago de Compostela, Galicia, Spain

4:30 - 4:50pm

330 Structural and Mechanistic Insights into Disease-associated Endolysosomal Exonucleases PLD3 and PLD4

Meng Yuan, Linghang Peng, Deli Huang, Amanda Gavin, Fangkun Luan, Jenny Tran, Ziqi Feng, Xueyong Zhu, Jeanne Matteson, Ian Wilson, David Nemazee

The Scripps Research Institute, La Jolla, California, USA

4.2.3 General Interest Part 3

2:00 - 5:00pm Thursday, 11th July, 2024
Conifer Ballroom
Zhen Xu, Tim Stachowski

General Interest sessions are the forum for topics of broad interest to the structural science or for presentations that do not fit the specific theme of other sessions. All presentations are selected from submitted abstracts.

2:00 - 2:20pm

290 New and Updated Features in Phenix for Macromolecular Structure Determination

Billy Poon

Lawrence Berkeley National Laboratory, Berkeley, CA, USA

2:20 - 2:40pm

111 What is the best target protein density for TELSAM fusion crystallization

Prasadika Samarawickrama Hetti Arachchige, James Moody

Brigham Young University, Provo, Utah, USA

2:40 - 3:00pm

105 Improving 1TEL-DARPin Crystallization via Linker Diversity Optimization for Enhanced Crystal Quality and Diffraction Data

Maria Pedroza, James Moody

Brigham Young Unviersity, Provo, Utah, USA

3:30 - 3:55pm

157 Bacterial Organelles: Encapsulation of Anaerobic Metabolic Pathways within Bacterial Microcompartments in the Human Microbiome

Lindsey Backman

Whitehead Institute for Biomedical Research, Cambridge, MA, USA

3:55 - 4:15pm

126 The occurrence of $^{Trp}C_{d1}$-H...O=$C^{backbone}$ hydrogen bonds in proteins

MIchal Sczygiel[1], Urszula Derewenda[2], Steve Scheiner[3], Wladek Minor[2], Zygmunt Derewenda[2]

[1]Jagiellonian University, Krakow, Lesser POland, Poland. [2]University of Virginia, Charlottesville, VA, USA. [3]Utah State University, Logan, UT, USA

4:15 - 4:35pm

165 Fuzzy interactions maintain cognate pairings in TA systems

Christina Bourne[1], Kevin Snead[1,2], Felipe Avelino da Costa Ferreira[1]

[1]University of Oklahoma, Norman, OK, USA. [2]Bayer, Chesterfield, MO, USA

4:35 - 5:00pm

17 Structure-guided design of SARS-CoV-2 PL^{pro} inhibitors with *in vivo* antiviral efficacy

Ahmadullah Ansari[1,2], Francesc Ruiz[1,2], Bin Tan[3,2], Xiaoming Zhang[4], Prakash Jadhav[3,2], Haozhou tan[3,2], Kan Li[3,2], Ashima Chopra[1,2], Alexandra Ford[4], Xiang Chi[4], Xufang Deng[4], Jun Wang[3,2], Eddy Arnold[1,2]

[1]Center for Advanced Biotechnology and Medicine, and Department of Chemistry and Chemical Biology, Piscataway, NJ, USA. [2]Rutgers University, Piscataway, NJ, USA. [3]Department of Medicinal Chemistry, Ernest Mario School of Pharmacy, Piscataway, NJ, USA. [4]Oklahoma State University, Stillwater, OK, USA

4.2.4 Super-charging experiments using real-time analysis: crystallography in the high data rate age

2:00 - 5:00pm Thursday, 11th July, 2024
Evergreen C
Johannes Blashke, Christine Beavers

Recent advances in detector design and photon flux have resulted in an exponential increase in the data rates produced by Synchrotrons and XFELs. This enables the experimenter to explore more ambitious measurements such as, fragment screening, phase transitions and time-resolution. At the same time, new data analysis algorithms have become more demanding in terms of total computational work, I/O, networking, GPUs and accelerator hardware. This requires thoughtful investment in IT infrastructure to handle increased data processing and storage, combined with efficient data analysis. This session brings together an interdisciplinary group for a wide ranging discussion on these topics that are typically overlooked but can be key to experimental success. We will highlight several recent high-data rate use cases, encountered challenges, and potential new solutions.

2:00 - 2:30pm

233 Real-time Data Analysis with the LCLS-II Data System

Valerio Mariani, Richard Claus, Daniel Damiani, Christopher Ford, Mikhail Dubrovin, Wilko Kroeger, Stefano Marchesini, Riccardo Melchiorri, Silke Nelson, Frederic Poitevin, Christopher O'Grady, Julieth Wallace, Omar Quijano, Murali Shankar, Monarin Uervirojnangkoorn, Matt Weaver, Seshu Yamajala, Cong Wang, Vincent Esposito, Jana Thayer

SLAC National Accelerator Laboratory, Menlo Park, California, USA

2:30 - 3:00pm

108 Recent Advances in Resonet: Towards Processing of Diffraction Data using Deep Residual Networks

Derek Mendez[1], James Holton[1,2,3], Artem Lyubimov[1], Aina Cohen[1]

[1]SLAC National Lab, Menlo Park, CA, USA. [2]Lawrence Berkeley National Lab, Berkeley, CA, USA. [3]UCSF, San Francisco, CA, USA

3:30 - 4:00pm

303 Progress in Computational Methods for XFEL Single-Particle 3D Nanoscale Imaging

Osamu Miyashita[1], Florence Tama[1,2,3]

[1]RIKEN Center for Computational Science, Kobe, Hyogo, Japan. [2]Department of Physics, Graduate School of Science, Nagoya University, Nagoya, Aichi, Japan. [3]Institute of Transformative Bio-Molecules, Nagoya, Aichi, Japan

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4:00 - 4:30pm

334 Scaling Scaling: Stochastic Variational Inference for X-ray Diffraction Data

Kevin Dalton[1,2,3], Doeke Hekstra[2]

[1]SLAC National Lab, Menlo Park, CA, USA. [2]Harvard Univeristy, Cambridge, MA, USA. [3]New York University, New York, NY, USA

4.2.5 Recent Advances in Fiber Diffraction

2:00 - 5:00pm Thursday, 11th July, 2024
Evergreen EF
Rama Sashank Madhurapantula, Joseph Orgel

This session explores the latest advancements in X-ray fiber diffraction methods and the insights gained into molecular structures using these developments. The session will host presentations from research performed in revolutionary technique development, biological, chemical and physical insights and how they correlate to material science, mathematical modeling and other interdisciplinary research areas. The talks will also showcase possible areas of collaboration of this rather niche research technique that is capable of delivering high acuity data into the aforementioned areas.

2:00 - 2:30pm

273 Musclex – DI – A powerful data analysis package for X-ray scanning diffraction experiments

Rama S. Madhurapantula[1], Joseph P.R.O. Orgel[1], Weikang Ma[1,2], Thomas Irving[1,2]

[1]Illinois Institute of Technologuy, Chicago, IL, USA. [2]Biophysics Collaborative Access Team, APS, ANL, Lemont, IL, USA

2:30 - 3:00pm

295 Density of the extracellular matrix in pancreatic cancer solid tumors has consequences on high molecular weight drug delivery

Cody Rounds, Sanzida Haque, Chengyue Li, Devin Nissen, Dhruv Ranjan, Marcell Vaicik, Rama Sashank Madhurapantula, Kenneth Tichauer

Illinois Institute of Technology, Chicago, IL, USA

3:30 - 4:00pm

267 Immune Interactions at the surface of tissue fibrils

Joseph Orgel, Rama Madhurapantula

Illinois Tech, Chicago, IL, USA

4:00 - 4:30pm

306 Understanding the structural characteristics of molecular assemblies in connective tissues

Olga Antipova[1], Joseph Orgel[2], Tom Irving[2], Stuart Stock[3], Jun-Sang Park[1]

[1]Argonne National Laboratory, Lemont, IL, USA. [2]Illinois Institute of Technology, Chicago, IL, USA. [3]Northwestern University, Chicago, IL, USA

4:30 - 5:00pm

282 The structural and functional integrities of porcine myocardium are mostly preserved by cryopreservation

Weikang Ma[1], Kyoung Hwan Lee[2], Christine Delligatti[3], M. Therese Davis[3], Yahan Zheng[4], Henry Gong[5], Jonathan Kirk[3], Roger Craig[6], Thomas Irving[1]

[1]BioCAT, Department of Biology, Illinois Institute of Technology, Chicago, IL, USA. [2]Electron Microscopy Facility, UMass Chan Medical School, Worcester, MA, USA. [3]Department of Cell and Molecular Physiology, Loyola University Chicago, Chicago, IL, USA. [4]College of Basic Medical Sciences, Dalian Medical University, Dalian, Lianning, China. [5]BioCAT, Department of Biology, Illinois Institute of Technology, Chicago, Il, USA. [6]Division of Cell Biology and Imaging, Department of Radiology, University of Massachusetts Medical School, Worcester, MA, USA

4.2.6 Biomolecular Dynamics & Frontiers in SAS

2:00 - 5:00pm Thursday, 11th July, 2024
Evergreen D
Tom Grant, Jesse Hopkins

The structural characterization of biomolecules is essential for understanding their function and the impact of environmental factors on their behavior. Small angle scattering (SAS) is an indispensable tool in structural biology and provides unique insights into the conformational changes, dynamics, and interactions of biomolecules in their native solution state. Recent advances in light sources, experimental methods and computational algorithms have enabled exciting new discoveries using SAS. This session is devoted to discussing the latest advances in methods and applications of X-ray and neutron SAS to biomolecular dynamics. The primary aim is to bring together cutting-edge advances utilizing SAS on both soft matter and biological systems, including time-resolved studies, contrast matching, dynamic and flexible systems, hybrid modeling, novel experimental apparatus and methods, and new computational approaches. This session brings together experts and researchers who have been at the forefront of pioneering work in structural biology, shedding light on the dynamic aspects of biological macromolecules.

2:00 - 2:30pm

31 Microsecond time-resolved X-ray scattering by utilizing MHz repetition rate at second-generation XFELs

Westenhoff Sebastian, Konold Patrick, Monrroy Leonardo, Maia Filipe

University of Uppsala, Uppsala, Uppsala, Sweden

2:30 - 3:00pm

36 Folding Dynamics of Telomere G-Quadruplexes: Insights from Time-Resolved SAXS and Biophysical Approaches

Robert Monsen, John Trent, Jonathan Chaires

University of Louisville, Louisville, Kentucky, USA

3:30 - 3:50pm

80 Predicting RNA structure and dynamics with deep learning and solution scattering

Edan Patt[1], Scott Classen[2], Dina Schneidman[1], Michal Hammel[2]

[1]The Hebrew University of Jerusalem, Jerusalem, Israel, Israel. [2]LBNL, Berkeley, CA, USA

3:50 - 4:10pm

55 Time-Resolved Pump-Probe X-Ray Solution Scattering Capabilities at BioCARS 14 ID Beamline, Advanced Photon Source.

Irina Kosheleva[1,2], Robert Henning[1,3], Insik Kim[1,2], Eric Zoellner[1,2], Vukica Srajer[1,3], Rama Ranganathan[1,2]

[1]The University of Chicago, Chicago, IL, USA. [2]Sector 14 BioCARS, APS, Argonne National Laboratory, Lemont, IL, USA. [3]Sector 14 BioCARS, APS, Argonne national Laboratory, Lemont, IL, USA

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4:10 - 4:30pm

91 Small-angle X-ray microdiffraction reveals the presence of sub-micron sized voids in fixed human brain tissue

Prakash Nepal, Abdullah Al Bashit, Lee Makowski

Northeastern University, Boston, MA, USA

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4:30 - 5:00pm

70 Resolving Structural Dynamics in Biological Macromolecules with Time-resolved X-ray Solution Scattering and Molecular Dynamics Simulation

Adam Nijhawan[1], Arnold Chan[1], Madeline Ho[1], Kevin Kohlstedt[1], Lin Chen[1,2]

[1]Northwestern University, Evanston, IL, USA. [2]Argonne National Laboratory, Lemont, IL, USA

All Members Business Meeting

5:15 - 6:15pm Thursday, 11th July, 2024
Evergreen A
Allen Oliver

Closing Celebration

6:30 - 10:30pm Thursday, 11th July, 2024
Rocky Mountain Event Center
Stacey Smith, Samantha Powell, Anna Gardberg, Sarah Bowman

Join us for an evening of camaraderie and reflection as we wrap up ACA2024. The Closing Celebration will feature dinner and drinks as well as awards and a chance to connect with fellow attendees in a relaxed and festive atmosphere. Meet us in the atrium for drinks at 6:30 PM and move to the Rocky Mountain Event Center for dinner at 7:00 PM.

2025 Planning Meeting

8:00am - 12:00pm Friday, 12th July, 2024
Conifer Ballroom
Sarah Bowman, Anna Gardberg, Samantha Powell, Stacey Smith