# 75th Annual Meeting of the American Crystallographic Association

**JULY 18-23, 2025 | LOMBARD, ILLINOIS**

# Table of Contents



If you would like to view the full abstract please see Structural Dynamics Volume 12, Issue 5_Supplement: https://pubs.aip.org/aca/sdy/issue/12/5_Supplement

# 75th ACA Annual Meeting

Schedule

## Thursday, 17 July, 2025

7:00-8:00pm Grand Ballroom Foyer

### Badge Pickup

If you arrive early on Thursday, 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 ACA2025.

## Friday, 18 July, 2025

7:30am-6:00pm Grand Ballroom Foyer

### Registration Desk

7:30am-5:00pm Walnut

### Speaker Ready Room

8:00am-5:30pm Lilac B

### WK1: An Introduction to Complementary Solution Biophysics for the Structural Biologist

Kushol Gupta, Maxwell Watkins
Sponsors: Rigaku, BioAnalysis

The workshop, An Introduction to Complementary Solution Biophysics for the Structural Biologist, at the 2025 ACA Annual Meeting will introduce participants to essential solution biophysics methods used in structural biology. These techniques are critical for understanding macromolecular properties such as mass, stoichiometry, shape, and thermodynamics, complementing traditional structural approaches like X-ray Crystallography, cryo-EM, and NMR. Through a mix of lectures and hands-on tutorials, attendees will gain practical knowledge of methods such as analytical ultracentrifugation, light scattering, and small-angle scattering. The workshop aims to provide a foundational understanding of these techniques, their applications, and how they validate macromolecular structures in a biologically relevant environment.

Attendees can expect a comprehensive, one-day learning experience that balances theoretical insights with hands-on applications. The workshop will cover fundamental solution biophysics concepts, introduce state-of-the-art techniques, and guide participants through practical exercises to analyze macromolecular properties. Experts in the field will deliver lectures and tutorials on topics such as hydrodynamic modeling, analytical ultracentrifugation, light scattering, and mass photometry. Additionally, attendees will have the opportunity to engage in discussions, receive feedback on their own data, and network with peers and industry professionals. The session is designed to be highly interactive, making it an excellent opportunity for students and early-career researchers to expand their structural biology toolkit.

8:30-10:00am Cypress A

### DEI-1A #IAmRemarkable - PREREGISTRATION REQUIRED

Alexis Davidson, Sandra Gabelli, Alice Thwin

#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

8:30-10:00am Cypress B

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8:45am-5:15pm Lilac A

## WK2: Applications of Visualization Technology in the Structural Sciences

Edward Eng, Nichole Valdez
Sponsors: NanoSoft, New England BioLabs, SubAngstrom

The Structural Science Visualization Technology Workshop at the Chicago ACA Meeting will focus on the latest advancements in visualization techniques for structural sciences, particularly in cryo-electron microscopy and X-ray crystallography. The workshop will cover cutting-edge visualization tools such as 2D and 3D molecular animations, virtual reality (VR), augmented reality (AR), and 3D printing to enhance the presentation and understanding of molecular structures. Attendees will engage in expert-led lectures, hands-on demonstrations, and discussions to explore how these technologies can be applied in scientific communication, education, and drug design.

Participants can look forward to an immersive learning experience where they will gain practical skills in using animation, VR, AR, and 3D printing to visualize complex structural data. The workshop will feature renowned experts from institutions such as the University of Utah, UC San Diego, and Schrödinger, offering insights into the latest tools like PyMOL3, syGlassVR, and Nanome.ai. Attendees will engage in interactive sessions, including hands-on demonstrations of 3D/4D visualization, molecular animations, and real-time virtual collaboration for chemical and pharmaceutical research. The event is ideal for scientists, educators, and students looking to enhance their ability to present structural data in innovative and compelling ways, making their research more accessible and impactful.

8:45am-5:00pm Lilac C

## WK4: Crystallographic and Cryo-EM Structure Solution with Phenix

Dorothee Liebschner

The Phenix workshop at ACA 2025 will focus on the structure determination of biological macromolecules using the Phenix software package. Phenix processes data from various diffraction methods and cryo-EM to derive macromolecular structures, emphasizing automation to reduce manual effort. The workshop will provide a combination of lectures and hands-on tutorials covering key aspects of structure solution, including initial model building, refinement, and validation. Special attention will be given to Phenix's tools for integrating AlphaFold-predicted models in crystallography and cryo-EM workflows. Attendees will engage in discussions and interactive tutorials led by Phenix developers, ensuring a comprehensive understanding of the software. The workshop also serves as a feedback platform for developers to enhance Phenix's usability.

Participants of this full-day workshop will gain practical experience in using Phenix for crystallographic and cryo-EM structure determination. The sessions will include lectures on key computational strategies, followed by hands-on tutorials covering model prediction, refinement, and validation. Attendees will have the unique opportunity to learn directly from Phenix developers, ask questions, and work through structured exercises designed to reinforce key concepts. By the end of the workshop, they will be equipped with the skills needed to efficiently use Phenix in their own research. Additionally, the event provides an excellent opportunity for networking with fellow researchers and software developers, fostering collaboration in the structural biology community.

1:00-5:30pm Cypress B

## WK3: Enhancing PDB Deposition and Validation Practices Workshop

Christine Zardecki
Sponsors: RCSB Protein Data Bank

The Enhancing PDB Deposition and Validation Practices workshop, organized by the RCSB Protein Data Bank (PDB), is designed to train researchers in efficient and accurate deposition of three-dimensional (3D) biostructure data. This interactive half-day event will focus on best practices for submitting structures obtained through X-ray crystallography, cryo-electron microscopy, and NMR spectroscopy. Through a mix of lectures and hands-on tutorials, participants will learn how to prepare necessary data files, validate structures using the Worldwide Protein Data Bank (wwPDB) OneDep system, and leverage key tools for improving submission efficiency. Attendees will leave with the expertise needed to confidently deposit and validate their 3D structures while ensuring high-quality data entry.

Participants can anticipate a practical and engaging workshop that blends instructional lectures with hands-on exercises. They will gain firsthand experience using the OneDep deposition system, learning step-by-step how to prepare, validate, and submit their 3D structures. The workshop will also introduce essential validation tools and best practices to ensure the accuracy of deposited data. Attendees will have the opportunity to interact with expert biocurators, receive personalized guidance, and discuss common challenges in PDB deposition. By the end of the session, participants will be well-equipped to efficiently submit and validate their structures, whether they are depositing for the first time or looking to refine their process.

5:30-6:00pm Lilac D

## Mentor/Mentee MeetUp

Gerald Audette

The mentor-mentee meetup is a dynamic and engaging opportunity for participants to connect, share experiences, and build meaningful professional relationships. If you signed up to be a mentor or mentee, this session is your chance to meet your conference partner in person and kick off your connection. Through open conversation and thoughtful guidance, mentors offer valuable insights from their own journeys, while mentees bring fresh perspectives and questions that spark rich dialogue. This welcoming environment is designed to foster collaboration, support, and growth for everyone involved.

6:30-7:30pm Junior Ballroom BC

Welcome & Key Note

It is with great enthusiasm that we welcome Stephen K. Burley, M.D., D.Phil., as the distinguished keynote speaker for the 2025 Annual Meeting of the American Crystallographic Association. A longtime and highly esteemed ACA member, Dr. Burley is an internationally recognized structural biologist, physician-scientist, and a leading figure in macromolecular crystallography. As the Director of the RCSB Protein Data Bank (PDB) and a Professor at Rutgers University, his pioneering work has profoundly advanced our understanding of protein structure, function, and its critical role in drug discovery.

7:30-10:00pm Exhibit Hall

Opening Reception

Saturday, 19 July, 2025

7:30am-5:00pm Grand Ballroom Foyer

Registration Desk

7:30am-5:00pm Walnut

Speaker Ready Room

8:30-11:30am Junior Ballroom C

TR1: Transactions I Evolving Landscape of Structural Science: AI and Multimethod Approaches

George Lountos, Krystle McLaughlin, Thomas Proffen, Carla Slebodnick
Sponsors: MiTeGen, Rigaku

8:30-11:30am Magnolia A

1.1.1 Serial/Multicrystal Protein Crystallography

Artem Lyubimov, Darya Marchany-Rivera
Sponsors: Dectris

Advances and updates to Multicrystal data collection and processing

8:30-11:30am Lilac AC

1.1.2 Advances in Membrane Protein Structural Biology

Susmith Mukund, Samantha Powell, Christina Rodriguez
Sponsors: Helix Biostructures, Gatan

Membrane proteins are some of the most difficult proteins to work with and are key proteins regulating intricate cellular control while themselves being drug targets. This session will focus on the structural biology of membrane proteins and recent technological advances in the field.

8:30-11:30am Magnolia BC

1.1.3 Crystallography Through the Decades

Ashfia huq, Cora Lind-Kovacs
Sponsors: Bruker AXS Inc, Dectris

In celebration of ACA's 75th anniversary, this session aims to highlight the tremendous contributions of structural sciences in a variety of fields over the past decades. We especially welcome talks on the progress of techniques in X-ray, Neutron, and electron crystallography over the past three-quarter century. In addition, contributions on transformative applications in the fields of chemistry, physics, materials science, biology and geology are encouraged. Presentations may provide a look back on our achievements or visions for cutting-edge structural science to envision for future decades to come.

8:30-11:30am Lilac B

1.1.4: Advances in Synchrotron-Based Characterization of Additive Manufacturing Processes & Properties

Hilmar Koerner, Arthur Woll
Sponsors: Dectris, GE Aerospace

The session will delve into recent developments and importance of synchrotron x-ray scattering techniques in elucidating the development of intra- and inter-layer structures in materials during additive manufacturing (AM). Additive manufacturing technologies are proving to disrupt various industries by enabling the creation of complex, high-performance components with unparalleled design freedom. However, the current state of the art faces significant challenges, particularly in achieving consistent material properties and optimal performance. One of the critical hurdles is understanding the complex interplay between processing parameters, structural formation at various length scales, and the resulting performance properties of the manufactured parts. Synchrotron X-ray techniques (e.g. scattering, diffraction, imaging) offer a powerful means to monitor and analyze the real-time evolution of material structures at various length scales during the AM process. This session will highlight recent advancements, provide insights into overcoming existing challenges, and discuss how these techniques can drive the development of more reliable and high-performance additive manufacturing processes.

8:30-11:30am Lilac D

## 1.1.5 General Interest I

Tim Stachowski, Zhen Xu
Sponsors: Rigaku, Bruker AXS Inc

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

11:45am-12:45pm Junior Ballroom C

## PL1 Etter Award: Dr. Dmitry Lyumkis

The ACA is proud to recognize Dr. Dmitry Lyumkis with the 2025 Margaret C. Etter Early Career Award for his groundbreaking contributions to structural biology and cryo-electron microscopy (cryo-EM). Dr. Lyumkis has advanced our understanding of infectious disease mechanisms, particularly HIV, through high-resolution structural insights into key viral protein complexes and their interactions with host cells.

A standout in both research and methodology, Dr. Lyumkis was among the first to resolve the structure of the HIV-1 envelope glycoprotein trimer, a pivotal breakthrough in vaccine development. His lab has since uncovered how viral intasomes integrate into host chromatin, how antiviral drugs block this process, and how resistance to therapy evolves. His innovations in cryo-EM, especially in overcoming sample preparation and validation challenges, have become widely adopted tools within the structural biology community.

Currently an Associate Professor at The Salk Institute and holder of the Hearst Foundations Chair, Dr. Lyumkis exemplifies the spirit of the Etter Award through his innovative science, leadership in the field, and profound impact on structural biology at large. We are honored to celebrate his achievements as a rising leader in the global scientific community.

12:45-1:45pm Magnolia A

## Three Minute Thesis

Kenneth Childers, Alexander Erickson

Join us for one of the most dynamic and engaging sessions of the conference—the Three Minute Thesis (3MT) competition! This fast-paced event challenges participants to present their research clearly and compellingly in just three minutes, using only one static slide. Whether you're competing or cheering from the audience, the 3MT is a great opportunity to discover cutting-edge work across the field, support your peers, and be inspired by the next generation of crystallographers. Don't miss it!

2:00-5:00pm Junior Ballroom C

## TR2: Transactions II Evolving Landscape of Structural Science: AI and Multimethod Approaches

George Lountos, Krystle McLaughlin, Thomas Proffen, Carla Slebodnick
Sponsors: MiTeGen, Rigaku

2:00-5:00pm Lilac D

## 1.2.1 Neutrons in Structural Biology

Gloria Borgstahl, Duminda Liurukara

Neutron scattering is a powerful tool to study the structure-function relationship of biomacromolecules and biomolecular complexes. Neutrons display a distinct sensitivity to the positions and motions of hydrogen atoms, the most abundant and elusive element found in biological systems, able to provide unique, complementary information to that gained from traditional structural biology techniques. Some capabilities of neutron scattering methods include that ability to locate individual hydrogen positions with atomic resolution, structural analysis of large-scale assemblies, and dynamics ranging from femto- to microsecond time scales. This session aims to highlight the exciting research benefiting from neutron-based structural techniques and bring attention to the advantages of using neutrons in structural biology.

2:00-5:00pm Magnolia A

## 1.2.2 MicroED for Small Molecules

Fernando Castro, Joseph Ferrara
Sponsors: Rigaku, Gatan, Dectris

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.

2:00-5:00pm Magnolia BC

1.2.3 Utilizing in Situ and Operando Techniques to Elucidate Complex Systems

Saul Lapidus, Cheng Li
Sponsors: Gatan

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.

2:00-5:00pm Lilac B

1.2.4 Crystallographic Data Analysis and Processing

Dominika Borek, Aaron Brewster
Sponsors: Dectris, Helix Biostructures, Bruker AXS Inc

This session focuses on methodologies and innovative techniques in the analysis and processing of crystallographic data. We are seeking contributions that present novel algorithms, software tools, and workflows that enhance the accuracy, efficiency, and robustness of data analysis in crystallography. Abstracts should cover topics such as data collection optimization, error reduction strategies, and data integration.

2:00-5:00pm Lilac AC

1.2.5 Innovations in Sample Preparation and other Hardware in CryoEM

Edward Eng, David Taylor
Sponsors: Structura Biotechnology Inc., Direct Electron, LP, Helix Biostructures, ThermoFisher, NanoSoft, MiTeGen

Developments in cryoEM and cryoET methods and technology have revolutionized our ability to see the atomic structure of proteins and biological macromolecules in the cellular environment. In this session, we explore and discuss new developments in sample preparation and EM technologies that address current challenges and open doors to exciting areas of biology.

5:30-7:30pm Exhibit Hall

PS1: Poster Session #1

Leighanne Gallington, Cora Lind-Kovacs, Tim Stachowski

Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don't miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

8:00-10:00pm Offsite: Millers Ale House

YSIG Mixer

Sponsors: Bruker AXS Inc

Join us on Saturday, July 19th at 8:00 PM CDT at Miller's Ale House (70 Yorktown Shopping Center, Lombard, IL 60148)—just a short distance from the hotel.
You're welcome to make your own way there, or hop on one of our complimentary shuttles departing from the front of The Westin Lombard Chicago at 7:45 PM, 8:00 PM, and 8:15 PM CDT. Return shuttles will leave Miller's Ale House at 9:45 PM, 10:00 PM, and 10:15 PM CDT.

Each guest will receive one drink ticket, with a cash bar available for additional beverages. We'll also be serving a selection of appetizers, including boneless wings, mini cheeseburgers, mozzarella sticks, fried potstickers, spinach artichoke dip, and gluten-free options. Please note: food will be served, but it is not intended to replace a full meal.

This is one of the most anticipated social events of the conference—don't miss the chance to connect with new and familiar colleagues in a fun, relaxed setting.

As always, please drink responsibly and make choices that ensure a safe and enjoyable evening for all.

## Sunday, 20 July, 2025

7:30am-5:00pm Grand Ballroom Foyer

Registration Desk

7:30am-5:00pm Walnut

Speaker Ready Room

8:30-11:30am Junior Ballroom C

## 2.1.1 Emerging Modalities for Pharma Part 1

Susmith Mukund, Elizabeth Sprague
Sponsors: Rigaku

This session will focus on the application of cryo-EM, x-ray crystallography and complementary biophysical and computational methods to the discovery and optimization of various drug modalities. For decades, small molecules by far have been the preferred modality to tackle diseases. While the past couple of decades have seen an exciting influx of transformative therapeutic antibodies, today, several other "non-standard" entities such as PROTACs, antibody-like scaffolds, macrocycles, peptides, covalent modulators, to name a few, are being developed to address unmet medical needs. We welcome submissions showcasing relevant structural biology techniques to drug discovery.

8:30-11:30am Magnolia A

## 2.1.2 Hot Structures

Chhandosee Ganguly, George Lountos, James Moody
Sponsors: Helix Biostructures, Hampton Research, Bruker AXS Inc

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, CryoEM, Small Angle X-ray Scattering, or hybrid methods including those that incorporate predictive / computational modeling.

8:30-11:30am Lilac AC

## 2.1.3 Innovations in Algorithms and Computational Methods

Joseph Davis, Alexis Rohou
Sponsors: Structura Biotechnology Inc., MiTeGen, Genetech, Inc., The McLellan Family, NanoSoft

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.

8:30-11:30am Magnolia BC

## 2.1.4 Crystal Engineering

Veronica Carta, Dan Decato

The intentional design and assembly of crystalline materials to control their physical and chemical properties (aka Crystal Engineering) is an interdisciplinary field. This session will encompass various experimental and theoretical topics centered on solid-state assembly including, but not limited to, supramolecular interactions, multicomponent crystal systems, polymorphism, and the mechanical properties of crystalline materials. The session aims to balance translational and fundamental studies showcasing the versatility and impact of crystal engineering across disciplines.

8:30-11:30am Lilac B

## 2.1.5 Applications, Advances and Challenges with Total Scattering for Disorder Studies

Danielle Alverson, Yuanpeng Zhang
Sponsors: Rigaku

Total scattering encompasses both Bragg and diffuse scattering, enabling data analysis and modeling to extract structural information from both an average and local perspective. Since the resurgence of total scattering in the late 1980s, there has been a continuous emphasis on studying local disorder in various functional materials. This session aims to showcase recent applications of total scattering in investigating local disorder in energy storage materials, catalysts, magnetic systems, and other areas of interest. Furthermore, the session will explore recent and future advancements and challenges in instrumentation, data processing, analysis methodologies, and software tools. As the total scattering community continues to expand, this platform seeks to foster education, communication, and envision the future of the field.

8:30-11:30am Lilac D

## 2.1.6 Combining experimental data with predicted models for structure determination

Rakhi Rajan, Christopher Williams
Sponsors: Dectris, Bruker AXS Inc

This session focuses on the integration of crystallographic data with predicted models obtained from AI-driven tools like AlphaFold and RosettaFold. Abstracts should highlight methodologies and best practices for combining experimental data and predicted models to improve the structure determination workflow. The session also welcomes case studies demonstrating the application and benefits of these combined techniques in resolving biological structures.

11:45am-12:45pm Junior Ballroom C

PL2 Robert Bau Award: Dr. Craig Brown

Dr. Craig M. Brown, NIST Fellow and Director of the Center for High-Resolution Neutron Scattering (CHRNS), has been named the recipient of the Kenneth N. Trueblood Award. This award recognizes exceptional contributions to chemical crystallography and honors the legacy of Professor Kenneth N. Trueblood's impact on structural science.

Dr. Brown leads the Structure and Dynamics of Materials team at the NIST Center for Neutron Research and serves as an Adjunct Professor of Chemical Engineering at the University of Delaware. His work focuses on the structural and dynamical characterization of energy-related materials, including applications in hydrogen storage and small molecule separations. He has published over 250 scientific papers and is widely recognized in the field.

Dr. Brown's collaborative research spans DOE national labs and academic institutions. His accolades include the NIST Samuel Wesley Stratton Award, the DOE Hydrogen and Fuel Cells Program R&D Award, the Neutron Scattering Society of America Science Prize, the Arthur S. Flemming Award, the Department of Commerce Silver Medal, and the Presidential Early Career Award for Scientists and Engineers (PECASE).

12:45-1:45pm Cypress A

DEI-2A #IAmRemarkable - PREREGISTRATION REQUIRED

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12:45-1:45pm Cypress B

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12:45-1:45pm Lilac B

Industry Sponsored Lunch & Learn (Ticket Required)

Join us for a special sponsored workshop hosted in partnership with Excillum, Proto, and DECTRIS. This engaging session will offer valuable insights and hands-on expertise from leaders in the field. *Please note: attendance is by invitation only.* Tickets are required and can be picked up directly from the booths of Excillum, Proto, or DECTRIS in the exhibit hall. Be sure to stop by early—space is limited and tickets will be distributed on a first-come, first-served basis.

2:00-5:00pm Junior Ballroom C

2.2.1 Emerging Modalities in Pharma Part 2

Susmith Mukund, Elizabeth Sprague

This session will focus on the application of cryo-EM, x-ray crystallography and complementary biophysical and computational methods to the discovery and optimization of various drug modalities. For decades, small molecules by far have been the preferred modality to tackle diseases. While the past couple of decades have seen an exciting influx of transformative therapeutic antibodies, today, several other "non-standard" entities such as PROTACs, antibody-like scaffolds, macrocycles, peptides, covalent modulators, to name a few, are being developed to address unmet medical needs. We welcome submissions showcasing relevant structural biology techniques to drug discovery.

2:00-5:00pm Magnolia BC

2.2.2 A Hitchhiker's Guide to Peer Review

Chun Hsing 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.

2:00-5:00pm Magnolia A

2.2.3 Extreme Biology: Probing the Conformational Landscape and Data Collection outside of Standard Practice

Silvia Russi, Vivian Stojanoff

Modern technologies have brought new capabilities that allow us to explore a range of crucial questions starting with how extreme environments drive molecular adaptation and influence biological function in adverse settings. By exposing biological samples to a range of stresses like extreme heat, pressure, or acidity, we can discover previously unknown molecular states and their functional consequences. The vast array of genomic information offers a readily available and invaluable resource for a systematic study of the molecular effects of extreme conditions

2:00-5:00pm Lilac B

## 2.2.4 General Interest II

Alexis Davidson, Andrew Howard, Matthew McLeod
Sponsors: Rigaku, Bruker AXS Inc

General Interest sessions provide a platform for topics of broad relevance to structural science or for presentations that do not align with the specific themes of other sessions. All presentations are chosen from submitted abstracts.

2:00-5:00pm Lilac D

## 2.2.5 Quantum Materials: Synthesis and Characterization

Yu Li, Duminda Liurukara, Keith Taddei
Sponsors: Bruker AXS Inc, Dectris

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.

2:00-5:00pm Lilac AC

## 2.2.6 From Cells to Atoms – using CryoEM Approaches to address Biological Questions

Benjamin Barad, Juan Du
Sponsors: The McLellan Family, NanoSoft, Direct Electron, LP, MiTeGen, ThermoFisher, Structura Biotechnology Inc., Genetech, Inc., Pfizer

The ability to determine 3D structures of biological systems has skyrocketed due to recent advances in cryoEM. This section will focus on the use of single-particle cryo-EM and cryo-electron tomography to understand the molecular basis of biological processes.

5:30-7:30pm Exhibit Hall

## PS2: Poster Session #2

Leighanne Gallington, Cora Lind-Kovacs, Tim Stachowski

Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don't miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

6:00-8:00pm Junior Ballroom B

## Fellows Reception INVITE ONLY

The ACA Fellows Reception is a special evening dedicated to recognizing the outstanding contributions of our Fellows to the field of crystallography. This event offers an opportunity for Fellows and invited guests to connect in an informal setting, celebrate achievements, and foster community within the ACA.

Light refreshments and hors d'oeuvres will be served. We encourage all ACA Fellows to attend and join us in honoring this distinguished group.

7:30-9:30pm Junior Ballroom C

## 2.3.1 Would You Publish This

Gerald Audette, Storm Dragonson, Scott Lee
Sponsors: Bruker AXS Inc

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!

8:00-10:00pm Magnolia A

## Bragg About It: Karaoke Night

Looking to unwind and have some fun? Join for a Karaoke & Board Games Night!

Whether you're ready to belt out your favorite power ballad, dominate in Codenames, or just hang out with fellow structural science enthusiasts, we've got something for you.

Come solo or bring your friends—everyone is welcome!

Monday, 21 July, 2025

7:30am-5:00pm Grand Ballroom Foyer

Registration Desk

7:30am-5:00pm Walnut

Speaker Ready Room

8:30-11:30am Lilac D

## 3.1.1 Managing High Data Rates in Structural Science

Christine Beavers, Vivian Stojanoff, Justyna Wojdyla
Sponsors: Rigaku, Dectris, MiTeGen

This session invites abstracts that address the challenges and solutions associated with handling large volumes of crystallographic data. We seek contributions that explore techniques for processing high data rates, data compression methods, and scalable storage solutions. We also welcome submissions on best practices for long-term data archiving, integration of automated systems, and the use of cloud-based platforms to manage high-throughput crystallographic experiments. Abstracts implementing FAIR principles of making crystallographic data Findable, Accessible, Interoperable, and Reusable (FAIR) to improve reproducibility in research are also welcomed. These contributions could explore strategies and tools for implementing FAIR principles in data archiving, including metadata standards, data sharing platforms, best practices for data documentation and case studies where FAIR data archiving has improved reproducibility.

8:30-11:30am Magnolia BC

## 3.1.2 General Interest III

Alexis Davidson, Zhen Xu
Sponsors: Bruker AXS Inc, Rigaku

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

8:30-11:30am Lilac B

## 3.1.3 Mathematical, Theoretical, and Computational Crystallography

Carolyn Brock, 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.

8:30-11:30am Magnolia A

## 3.1.4 Quantum Crystallography: Latest Developments, Applications, and Experiences

Anna Krawczuk, Sylwia Pawledzio
Sponsors: Rigaku, Stoe, OlexSys, Dectris, MiTeGen, Bruker AXS Inc

This session is open to all scientists, from hands-on practitioners to experts in method development, and especially welcomes end-users of quantum crystallographic techniques to present their experiences and findings. Topics may encompass any theoretical or practical applications of quantum mechanics in the study of crystalline materials. Presenters are encouraged to demonstrate how these techniques enhance agreement with experimental data, leading to deeper material insights. Research areas can include inorganic solids, molecular networks, organic and organometallic compounds, as well as large structures like proteins.

8:30-11:30am Junior Ballroom C

## 3.1.5 Flexibility, Dynamics & The Secret Lives of Proteins

Marcus Fischer, Tim Stachowski, Kara Zielinski
Sponsors: St. Jude Children's Research Hospital

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.

8:30-11:30am Lilac AC

## 3.1.6 Developments in Data Collection and Automation in MicroED

Brandon Mercado, Shao-Liang Zheng
Sponsors: Quantum Detectors, Rigaku

MicroED has been at the forefront of expanding the possibilities of structure models accessible through crystallography. Numerous efforts have been dedicated to enhancing the pipeline for delivering these results. This session will explore advancements in automation, covering a wide range of topics. We will delve into general improvements in data collection strategies, as well as groundbreaking developments in truly autonomous, high-throughput approaches to MicroED. Additionally, we will discuss simultaneous compositional analysis of complex samples, further broadening the capabilities of MicroED. Join us in this session to discover the latest automation advances in microcrystal electron diffraction.

11:45am-12:45pm Junior Ballroom C

## PL3 Fankuchen Award: Professor Chris D. Malliakas

Chris D. Malliakas will receive the ACA Fankuchen Memorial Award in recognition of his significant contributions to crystallographic research and his dedication to teaching in the field. As the Director of Crystallography, Director of Physical Characterization, and Research Associate Professor at the Integrated Molecular Structure Education and Research Center (IMSERC) at Northwestern University, Malliakas has demonstrated expertise in solving complex structural problems, including modulated structures, amorphous compounds, supercells, twinning, and disorders. His work extends beyond single-crystal analysis, having transformed structural elucidation capabilities at Northwestern University into a dynamic learning environment where he actively trains future structural scientists. His dedication to both advancing crystallographic methodologies and educating the next generation of researchers exemplifies the essence of the Fankuchen Award, which honors those who contribute to crystallographic research while being effective educators.

11:45am-1:45pm Cypress A

## Private Event-Murphy

12:00-5:00pm Junior Ballroom B

## APS Site Visit - PREREGISTRATION REQUIRED

Important Note:
Only participants who meet all of the following criteria will be permitted to enter Argonne National Laboratory:

*Are registered with the ACA
*Have completed all required APS security steps
*Arrive and depart using the ACA-provided transportation
*Present a REAL ID-compliant driver's license or a valid passport at the security checkpoint

Schedule & Transportation

PLEASE MEET PROMPTLY AT 12:00 PM IN JUNIOR BALLROOM B

12:30 PM – 12:45 PM – Load buses at The Westin Chicago Lombard
*(70 Yorktown Shopping Center, Lombard, IL 60148)*
*A boxed lunch will be provided before departure.*
12:45 PM – 1:15 PM – Travel to Argonne National Laboratory *(Northgate Rd & South Cass Ave)*
1:15 PM – 2:00 PM – Security clearance and ID check at the main gate
(*REAL ID or valid passport required*)
2:00 PM – 2:15 PM – Arrive at APS, divide into groups, meet guides
2:15 PM – 2:30 PM – Welcome remarks by Jonathan Lang and Stefan Vogt
2:45 PM – 3:45 PM
4:00 PM – 5:00 PM
5:00 PM – 5:15 PM – Load buses
5:15 PM – 5:45 PM – Return to The Westin Chicago Lombard
Please remember to bring your conference badge, government-issued ID, and any personal items you may need.

5:30-7:30pm Exhibit Hall

## PS3: Poster Session #3

Leighanne Gallington, Cora Lind-Kovacs, Tim Stachowski

Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don't miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

7:30-8:15pm Junior Ballroom C

## All Members Business Meeting

8:15-9:15pm Junior Ballroom B

SIG Mixer

Tuesday, 22 July, 2025

7:30-11:00am Grand Ballroom Foyer

Registration Desk

8:30-11:30am Lilac AC

4.1.2 Structure of Nucleic Acids

Peter Hsu, Melanie Ohi
Sponsors: Structura Biotechnology Inc., Direct Electron, LP, NanoSoft, ThermoFisher, The McLellan Family, MiTeGen

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.

8:30-11:30am Magnolia A

4.1.3 Ab initio Designed Proteins

Jack Nicoludis, Vardhan Satalkar

New advancements in machine learning have recently and remarkably improved our ability to predict and design proteins. This session will explore the exciting field of protein design, where computational and experimental methods combine to engineer proteins with tailored structures and functions. A wide variety of topics will be covered, such as advancements in AI/ML methods in protein structure prediction and design, directed evolution and rational design, structural characterization of designed proteins, and applications of protein design, such as in synthetic biology, biomedical imaging, and drug discovery. The program is designed to address not only the technical challenges associated with protein design but also to enhance understanding of the relationship between protein structure, function, and dynamics, thereby expanding their range of applications in translational research.

8:30-11:30am Lilac D

4.1.4 Cool Structures

Kamran Ghiassi, Nichole Valdez
Sponsors: Helix Biostructures

8:30-11:30am Magnolia BC

4.1.5 Cryo-EM facilities: How to integrate multiple modalities on one instrument

Tamir Gonen, Brent Nannenga
Sponsors: The McLellan Family, Direct Electron, LP, Helix Biostructures, MiTeGen, Viva Biotech, Calico

The use of cryo-EM is expanding with several techniques including single particle cryo-EM, MicroED, and cryo-electron tomography using the same instrumentation. Many institutions are adding these technique to their suite of structure determination methods.This session will focus on experiences integrating and applying the different modalities of cryo-EM, and the best practices to ensure that all cryo-EM methods can coexist.

8:30-11:30am Lilac B

4.1.6 Fibers and Friends: X-ray Vision for Unmasking the Culprits in Neurodegenerative Disease

Olga Antipova, Rama Sashank Madhurapantula, Joseph Orgel

11:45am-12:45pm Junior Ballroom C

PL4 Trueblood Award: Professors Branton J. Campbell & Harold T. Stokes

Professors Branton J. Campbell and Harold T. Stokes of Brigham Young University have been named recipients of the Robert Bau Neutron Diffraction Award. This award honors outstanding accomplishments in the field of neutron diffraction and commemorates the legacy of Professor Robert Bau's impact on structural science.

Together, Professors Campbell and Stokes have made foundational contributions to the use of symmetry-mode analysis in interpreting neutron diffraction data. Their development of the ISOTROPY Software Suite, including tools like ISODISTORT and FINDSYM, has transformed how crystallographers characterize structural phase transitions — particularly in complex magnetic and functional materials.

Dr. Campbell's research integrates neutron powder and single-crystal diffraction techniques to explore structure-property relationships, while Dr. Stokes has led the crystallographic community in developing group-theoretical methods essential to symmetry analysis. Their decades-long collaboration has empowered researchers worldwide through accessible, rigorous computational tools and has advanced standards in magnetic structure communication.

12:45-1:55pm Cypress A

DEI-3A #IAmRemarkable - PREREGISTRATION REQUIRED

Alexis Davidson, Sandra Gabelli, Alice Thwin

#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

12:45-1:55pm Cypress B

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12:45-1:45pm Magnolia A

Career Odysseys/Career Panel

Melanie Adams-Cioaba, Edward Pryor

Join us for an engaging discussion as experienced industrial scientists share their personal journeys, challenges, and triumphs in the field. What makes a career in industry fulfilling? What key decisions shape professional growth and satisfaction? This session offers valuable insights for scientists at all stages, with a special focus on guidance for early-career professionals. Gain practical advice, explore diverse career paths, and learn what it takes to build a rewarding and impactful career in industrial science.

2:00-5:00pm Junior Ballroom C

4.2.1 AI/ML in Modern Structural Science

Emre Brookes, Debanu Das, Daniel Olds

The rapid advancements in artificial intelligence (AI) and machine learning (ML) are revolutionizing various scientific domains, including materials science, chemistry, physics, biology, and others. This session aims to explore how AI and ML techniques can be utilized in structural science in applications ranging from data analysis, structure determination, structure-based drug discovery and materials characterization to facility operation and sample throughput.
Submissions from all areas of structural science are welcome and could discuss challenges in AI/ML integration, present novel algorithms, or offer solutions for specific situations. Part 1 will focus on AI/ML applications to materials systems while Part 2 will focus on AI/ML applications to biological systems.

2:00-5:00pm Lilac AC

4.2.2 Small Molecule Crystal Structures for Pharmaceutical Development

Luca Iuzzolino, Justin Newman
Sponsors: Rigaku, Helix Biostructures, Bruker AXS Inc

Understanding the various properties of active pharmaceutical ingredients (APIs), including but not limited to physical, chemical, thermodynamic, kinetic, spectroscopic, mechanical, and surface properties, is of utmost importance to ensure a robust and reliable manufacture of small molecule drug products. This session aims to explore the ways that structure elucidation can impact our understanding of solid state properties and how they influence the manufacture of a robust drug product. Potential topics for this session could include drug substance form selection, properties (chemical or physical), polymorphism, and how these can potentially impact the design of a final drug product.

2:00-5:00pm Magnolia A

4.2.3 Engaging Students with Crystallography

Susanna Huang, Yinka Olatunji-Ojo, Joe Tanski
Sponsors: Bruker AXS Inc

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

2:00-5:00pm Magnolia BC

## 4.2.4 MicroED for Macromolecules and Drug Discovery

Johan Hattne, Mike Martynowycz
Sponsors: Rigaku

Building on the interplay between cutting-edge electron microscopy and minuscule crystal sizes, Microcrystal Electron Diffraction (MicroED) has become an indispensable tool for high-resolution structure determination of biological macromolecules and drug discovery. This session delves into unveiling newly determined macromolecular and new pharmaceutical structures facilitated by MicroED. 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 and drug discovery.

2:00-5:00pm Lilac D

## 4.2.5 SAS In Integrative Structural Approaches

Robert Monsen, Alexander Yarawsky
Sponsors: Rigaku

This session will showcase recent advancements in leveraging small-angle scattering (SAS) data in combination with orthogonal biophysical, biochemical, and computational methods to elucidate complex biological structures that are challenging for traditional approaches like X-ray diffraction, NMR, or cryo-EM. The examples will include, but are not limited to, studies on higher-order molecular assemblies, their structures, and dynamics. The focus will be on how these integrative models enhance our understanding of the spatio-temporal environment of the human cell.

2:00-5:00pm Lilac B

## 4.2.6 Structural Characterizations of Emerging Energy Materials

Si Athena Chen, Hao Liu
Sponsors: NanoSoft, MiTeGen, Direct Electron, LP, The McLellan Family

Structural characterizations of the next-generation energy materials are crucial for establishing precise relationships between chemistry, synthesis procedures, performance, and stability. This session invites works that apply in-depth structural characterizations on emerging energy materials for applications such as batteries, fuel cells, photovoltaics, thermoelectrics, piezoelectric devices, etc. Submissions may be steady-state or time-resolved structural studies of crystalline or amorphous energy materials, to understand the phase evolution during synthesis, structure-property relationships, degradation mechanisms, and other related aspects.

5:00-10:00pm Offsite: City Cruises – Spirit of Chicago

## Closing Celebration

Christine Beavers, Sarah Bowman, Samantha Powell, Stacey Smith

Reception Location
City Cruises – Spirit of Chicago
600 E Grand Ave, Chicago, IL 60611

Look for the “Spirit of Chicago” vessel docked at Navy Pier.

Schedule & Transportation

- 5:00 PM – Bus departs from the Westin Chicago Lombard
(70 Yorktown Shopping Center, Lombard, IL 60148)
final boarding is at 5:15 PM

If you miss the bus, you will need to arrange your own transportation to Navy Pier.

- 6:00 PM – Boarding begins at Navy Pier
- 6:30 PM – Boat launches and dinner begins
- 7:15 PM (approx.) – Closing remarks by ACA President Gerald Audette, awards presentations, and recognition of session chairs
- 9:30 PM – Boat returns to dock
- 10:00 PM – Return bus departs from Navy Pier back to the Westin
- 10:30 PM – Expected arrival at the Westin

Guests will enjoy a vibrant buffet dinner featuring entrées like citrus herb salmon, birria-style chicken, and spring garlic cream pasta—alongside fresh salads, seasonal sides, and a dessert station. Gluten-free, vegetarian, and some vegan options will be available.

Please wear your badge and bring any personal items you’ll need for the evening.

Wednesday, 23 July, 2025

9:00am-5:00pm Lilac A

## HDRMX workshop: Data Rates and Metadata over the Next Decade

Aaron Brewster, Graeme Winter
Sponsors: Dectris, Rigaku

HDRMX (High Data Rate Macromolecular Crystallography) is a consortium of interested software developers, detector manufacturers, facility staff, beamline scientists, and users, who meet to discuss next-generation challenges in data acquisition, transfer, processing, storage, and provenance.

This full-day session will consist of short talks and longer discussion sections, featuring topics such as anticipated data rates, the necessary infrastructure for transfer and processing, plans for long-term storage, benefits and difficulties with lossy compression, metadata standards, and deficiencies, multi-modal experiments, an provenance for raw data, processing, and deposition.

**Badge Pickup**
7:00 - 8:00pm Thursday, 17th July, 2025
Session Room: Grand Ballroom Foyer
If you arrive early on Thursday, 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 ACA2025.

**Registration Desk**
7:30am - 6:00pm Friday, 18th July, 2025
Session Room: Grand Ballroom Foyer

**Speaker Ready Room**
7:30am - 5:00pm Friday, 18th July, 2025
Session Room: Walnut

**WK1: An Introduction to Complementary Solution Biophysics for the Structural Biologist**
8:00am - 5:30pm Friday, 18th July, 2025
Session Room: Lilac B
Chairs Kushol Gupta, Maxwell Watkins
The workshop, An Introduction to Complementary Solution Biophysics for the Structural Biologist, at the 2025 ACA Annual Meeting will introduce participants to essential solution biophysics methods used in structural biology. These techniques are critical for understanding macromolecular properties such as mass, stoichiometry, shape, and thermodynamics, complementing traditional structural approaches like X-ray Crystallography, cryo-EM, and NMR. Through a mix of lectures and hands-on tutorials, attendees will gain practical knowledge of methods such as analytical ultracentrifugation, light scattering, and small-angle scattering. The workshop aims to provide a foundational understanding of these techniques, their applications, and how they validate macromolecular structures in a biologically relevant environment.

Attendees can expect a comprehensive, one-day learning experience that balances theoretical insights with hands-on applications. The workshop will cover fundamental solution biophysics concepts, introduce state-of-the-art techniques, and guide participants through practical exercises to analyze macromolecular properties. Experts in the field will deliver lectures and tutorials on topics such as hydrodynamic modeling, analytical ultracentrifugation, light scattering, and mass photometry. Additionally, attendees will have the opportunity to engage in discussions, receive feedback on their own data, and network with peers and industry professionals. The session is designed to be highly interactive, making it an excellent opportunity for students and early-career researchers to expand their structural biology toolkit.

**DEI-1A #IAmRemarkable - PREREGISTRATION REQUIRED**
8:30 - 10:00am Friday, 18th July, 2025
Session Room: Cypress A
Chairs Alexis Davidson, Alice Thwin, Sandra Gabelli
#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

**DEI-1B #IAmRemarkable - PREREGISTRATION REQUIRED**
8:30 - 10:00am Friday, 18th July, 2025
Session Room: Cypress B
Chairs Alexis Davidson, Alice Thwin, Sandra Gabelli
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**WK2: Applications of Visualization Technology in the Structural Sciences**
8:45am - 5:15pm Friday, 18th July, 2025
Session Room: Lilac A
Chairs Nichole Valdez, Edward Eng
The Structural Science Visualization Technology Workshop at the Chicago ACA Meeting will focus on the latest advancements in visualization techniques for structural sciences, particularly in cryo-electron microscopy and X-ray crystallography. The workshop will cover cutting-edge visualization tools such as 2D and 3D molecular animations, virtual reality (VR), augmented reality (AR), and 3D printing to enhance the presentation and understanding of molecular structures. Attendees will engage in expert-led lectures, hands-on demonstrations, and discussions to explore how these technologies can be applied in scientific communication, education, and drug design.

Participants can look forward to an immersive learning experience where they will gain practical skills in using animation, VR, AR, and 3D printing to visualize complex structural data. The workshop will feature renowned experts from institutions such as the University of Utah, UC San Diego, and Schrödinger, offering insights into the latest tools like PyMOL3, syGlassVR, and Nanome.ai. Attendees will engage in interactive sessions, including hands-on demonstrations of 3D/4D visualization, molecular animations, and real-time virtual collaboration for chemical and pharmaceutical research. The event is ideal for scientists, educators, and students looking to enhance their ability to present structural data in innovative and compelling ways, making their research more accessible and impactful.

**WK4: Crystallographic and Cryo-EM Structure Solution with Phenix**
8:45am - 5:00pm Friday, 18th July, 2025
Session Room: Lilac C
Chairs Dorothee Liebschner
The Phenix workshop at ACA 2025 will focus on the structure determination of biological macromolecules using the Phenix software package. Phenix processes data from various diffraction methods and cryo-EM to derive macromolecular structures, emphasizing automation to reduce manual effort. The workshop will provide a combination of lectures and hands-on tutorials covering key aspects of structure solution, including initial model building, refinement, and validation. Special attention will be given to Phenix’s tools for integrating AlphaFold-predicted models in crystallography and cryo-EM workflows. Attendees will engage in discussions and interactive tutorials led by Phenix developers, ensuring a comprehensive understanding of the software. The workshop also serves as a feedback platform for developers to enhance Phenix's usability.

Participants of this full-day workshop will gain practical experience in using Phenix for crystallographic and cryo-EM structure determination. The sessions will include lectures on key computational strategies, followed by hands-on tutorials covering model prediction, refinement, and validation. Attendees will have the unique opportunity to learn directly from Phenix developers, ask questions, and work through structured exercises designed to reinforce key concepts. By the end of the workshop, they will be equipped with the skills needed to efficiently use Phenix in their own research. Additionally, the event provides an excellent opportunity for networking with fellow researchers and software developers, fostering collaboration in the structural biology community.

**WK3: Enhancing PDB Deposition and Validation Practices Workshop**
1:00 - 5:30pm Friday, 18th July, 2025
Session Room: Cypress B
Chairs Christine Zardecki
The Enhancing PDB Deposition and Validation Practices workshop, organized by the RCSB Protein Data Bank (PDB), is designed to train researchers in efficient and accurate deposition of three-dimensional (3D) biostructure data. This interactive half-day event will focus on best practices for submitting structures obtained through X-ray crystallography, cryo-electron microscopy, and NMR spectroscopy. Through a mix of lectures and hands-on tutorials, participants will learn how to prepare necessary data files, validate structures using the Worldwide Protein Data Bank (wwPDB) OneDep system, and leverage key tools for improving submission efficiency. Attendees will leave with the expertise needed to confidently deposit and validate their 3D structures while ensuring high-quality data entry.

Participants can anticipate a practical and engaging workshop that blends instructional lectures with hands-on exercises. They will gain firsthand experience using the OneDep deposition system, learning step-by-step how to prepare, validate, and submit their 3D structures. The workshop will also introduce essential validation tools and best practices to ensure the accuracy of deposited data. Attendees will have the opportunity to interact with expert biocurators, receive personalized guidance, and discuss common challenges in PDB deposition. By the end of the session, participants will be well-equipped to efficiently submit and validate their structures, whether they are depositing for the first time or looking to refine their process.

**Mentor/Mentee MeetUp**
5:30 - 6:00pm Friday, 18th July, 2025
Session Room: Lilac D
Chairs Gerald Audette
The mentor-mentee meetup is a dynamic and engaging opportunity for participants to connect, share experiences, and build meaningful professional relationships. If you signed up to be a mentor or mentee, this session is your chance to meet your conference partner in person and kick off your connection. Through open conversation and thoughtful guidance, mentors offer valuable insights from their own journeys, while mentees bring fresh perspectives and questions that spark rich dialogue. This welcoming environment is designed to foster collaboration, support, and growth for everyone involved.

**Welcome & Key Note**
6:30 - 7:30pm Friday, 18th July, 2025
Session Room: Junior Ballroom BC
It is with great enthusiasm that we welcome Stephen K. Burley, M.D., D.Phil., as the distinguished keynote speaker for the 2025 Annual Meeting of the American Crystallographic

Association.  A longtime and highly esteemed ACA member, Dr. Burley is an internationally recognized structural biologist, physician-scientist, and a leading figure in macromolecular crystallography. As the Director of the RCSB Protein Data Bank (PDB) and a Professor at Rutgers University, his pioneering work has profoundly advanced our understanding of protein structure, function, and its critical role in drug discovery.

**Opening Reception**
7:30 - 10:00pm Friday, 18th July, 2025
Session Room: Exhibit Hall

**Registration Desk**
7:30am - 5:00pm Saturday, 19th July, 2025
Session Room: Grand Ballroom Foyer

**Speaker Ready Room**
7:30am - 5:00pm Saturday, 19th July, 2025
Session Room: Walnut

**TR1: Transactions I Evolving Landscape of Structural Science: AI and Multimethod Approaches**
8:30 - 11:30am Saturday, 19th July, 2025
Session Room: Junior Ballroom C
Chairs Thomas Proffen, George Lountos, Krystle McLaughlin, Carla Slebodnick

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8:30 - 9:00am
**395 AI at your service: AI tools for solving crystallographic problems**
Professor Simon J. L. Billinge PhD
Columbia University, New York, NY, USA

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9:00 - 9:30am
**207 Serial crystallography is just getting started**
Aaron S Brewster, Daniel W Paley, David W Mittan-Moreau, Nicholas K Sauter
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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9:30 - 10:00am
**49 Quantum Crystallography: Exploring Electron Density and Interactions**
Dr. Sylwia Pawledzio PhD, Dr. Xioping Wang PhD
Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

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10:30 - 11:00am
**300 Accelerating Crystal Structure Prediction with Machine Learning Forcefields**
Aaron D Kaplan PhD
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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11:00 - 11:30am
**221 Done before needed: The infrastructure that made crystallography so popular for machine learning**
Dr. Brian H Toby

Argonne National Lab, Lemont, IL, USA

**1.1.1 Serial/Multicrystal Protein Crystallography**
8:30 - 11:30am Saturday, 19th July, 2025
Session Room: Magnolia A
Chairs Darya Marchany-Rivera, Artem Lyubimov
Advances and updates to Multicrystal data collection and processing

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8:35 - 8:55am
**288 Returning to scientific operations at GM/CA@APS after the APS-Upgrade**
David J Kissick[1], Michael Becker[1], Stephen Corcoran[1], Dale Ferguson[1], Mark Hilgart[1], Oleg Makarov[1], Sergey Stepanov[1], Nagarajan Venugopalan[1], Qingping Xu[1], Shenglan Xu[1], Janet L Smith[2], Robert F Fischetti[1]
[1]Argonne National Laboratory, Lemont, IL, USA. [2]University of Michigan, Ann Arbor, MI, USA

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8:55 - 9:15am
**270 Multicrystal data collection at the VMXm beamline at Diamond Light Source**
Dr Anna J Warren[1], Dr Jose Trincao[1], Dr Adam D Crawshaw[1], Graham Duller[1], Dr Gwyndaf Evans[1,2]
[1]Diamond Light Source, Didcot, Oxfordshire, United Kingdom. [2]Rosalind Franklin Institute, Didcot, Oxfordshire, United Kingdom

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9:15 - 9:35am
**135 Closing the Gap - Integrated Time-Resolved Crystallography at the SwissFEL and Swiss Light Source**
Dr. Florian Dworkowski PhD
Paul Scherrer Institut, Villigen PSI, Aargau, Switzerland

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9:35 - 10:00am
**229 Capturing macromolecular dynamics using time-resolved serial crystallography at X-ray free electron lasers and synchrotron light sources**
Sandra Mous[1], Guillaume Gotthard[2], David Ehrenberg[3], Saumik Sen[2], Tobias Weinert[2], Philip Johnson[2], Daniel James[2], Karol Nass[2], Antonia Furrer[2], Pikyee Ma[2], Steffen Bruenle[2], Cecilia Casadei[2], Isabelle Martiel[2], Florian Dworkowski[2], Dardan Gashi[2], Petr Skopintsev[2,4], Maximilian Wranik[2,5], Gregor Knopp[2], Ezequiel Panepucci[2], Valerie Panneels[2], Claudio Cirelli[2], Dmitry Ozerov[2], Gebhard Schertler[2], Meitian Wang[2], Chris Milne[2], Joerg Standfuss[2], Igor Schapiro[6], Joachim Heberle[3], Przemyslaw Nogly[7]
[1]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [2]Paul Scherrer Institute, Villigen, AG, Switzerland. [3]Freie Universität Berlin, Berlin, BE, Germany. [4]University of California, Berkeley, CA, USA. [5]Stanford University, Palo Alto, CA, USA. [6]Hebrew University of Jerusalem, Jerusalem, JM, Israel. [7]Jagiellonian University, Krakow, MA, Poland

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10:30 - 10:55am
**290 Room-temperature X-ray fragment screening with serial crystallography**
Dr Sebastian Guenther, Alke Meents

DESY, Hamburg, Hamburg, Germany

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10:55 - 11:20am

**129 Cows, Pigs and People: Enhanced Intensity-Based Clustering of Isomorphous Multi-Crystal Datasets in the Presence of Subtle Variations**

Amy J Thompson[1], James Beilsten-Edmands[1], Cicely Tam[1,2,3], Juan Sanchez-Weatherby[1,2], James Sandy[1], Halina Mikolajek[1,2], Danny Axford[1], Sofia Jaho[1,2], Michael A Hough[1,2], Graeme Winter[1,4,5]

[1]Diamond Light Source, Didcot, Oxfordshire, United Kingdom. [2]Research Complex at Harwell, Didcot, Oxfordshire, United Kingdom. [3]University of Birmingham, Edgbaston, Birmingham, United Kingdom. [4]NE-CAT APS, Lemond, IL, USA. [5]Cornell University, Ithaca, NY, USA

**1.1.2 Advances in Membrane Protein Structural Biology**

8:30 - 11:30am Saturday, 19th July, 2025

Session Room: Lilac AC

Chairs Christina Rodriguez, Susmith Mukund, Samantha Powell

Membrane proteins are some of the most difficult proteins to work with and are key proteins regulating intricate cellular control while themselves being drug targets. This session will focus on the structural biology of membrane proteins and recent technological advances in the field.

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8:30 - 8:55am

**275 Structural insights into G protein-coupled receptor signaling**

Andrew Kruse

Harvard Medical School, Boston, MA, USA

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8:55 - 9:15am

**114 cryoEM structure of NINJ1, a small cytotoxic membrane protein.**

Ishan Deshpande

Genentech, South San Francisco, CA, USA

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9:15 - 9:35am

**119 *Regulation of ATP-Dependent Proteolysis by Membrane-Anchored Assemblies***

Dr. Alireza Ghanbarpour PhD[1], Dr. Naseer Iqbal[2]

[1]Washington University School of Medicine, St. Louis,, MO, USA. [2]Washington University School of Medicine, St. Louis, MO, USA

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9:35 - 10:00am

**366 Towards high-resolution *in-situ* structural biology of membrane protein complexes**

Rilee Zeinert[1], Madolyn Britt[2], Elissa Moller[1], Fei Zhou[1], Alexander Sodt[1], Gisela Storz[1], Sergei Sukharev[3], Doreen Matthies[1]

[1]Eunice Kennedy Shriver National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD, USA. [2]unice Kennedy Shriver National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD, USA. [3]Department of Biology, University of Maryland, College Park, MD, USA

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10:30 - 10:50am

**48 In the field of membrane protein structural biology, chance only favors the sample which is properly prepared**
Vikas Navratna PhD
University of Michigan, Ann Arbor, MI, USA

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10:50 - 11:10am
**268 MicroED for GPCRs**
Anna Shiriaeva Ph.D.
UCLA, Los Angeles, CA, USA

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11:10 - 11:30am
**256 Inhibition of Voltage-Gated Sodium Channels by Animal Toxins**
Assistant Professor Shane Gonen Ph.D.
UC Irvine, Irvine, CA, USA

**1.1.3 Crystallography Through the Decades**
8:30 - 11:30am Saturday, 19th July, 2025
Session Room: Magnolia BC
Chairs Cora Lind-Kovacs, Ashfia huq
In celebration of ACA's 75th anniversary, this session aims to highlight the tremendous contributions of structural sciences in a variety of fields over the past decades. We especially welcome talks on the progress of techniques in X-ray, Neutron, and electron crystallography over the past three-quarter century. In addition, contributions on transformative applications in the fields of chemistry, physics, materials science, biology and geology are encouraged. Presentations may provide a look back on our achievements or visions for cutting-edge structural science to envision for future decades to come.

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8:35 - 9:00am
**29 The Path of an Industrial Powder Small-Molecule Crystallographer**
James A Kaduk PhD
North Central College, Naperville, IL, USA

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9:00 - 9:20am
**362 Crystallography: 1970 – 2025 and Beyond**
Professor Carolyn P Brock PhD
University of Kentucky, Lexington, KY, USA

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9:20 - 9:40am
**237 Single-Crystal Diffraction at ORNL: Historical Development, Current Advances, and Future Perspectives**
Xiaoping Wang
Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

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9:40 - 10:00am
**324 On the power and promise of resonant diffraction for powders**
Dr. Kevin H. Stone, Dr. Sikhumbuzo M. Masina
SLAC National Accelerator Laboratory, Menlo Park, CA, USA

10:30 - 10:55am
**327 CryoEM milestones and future directions**
Professor Tamir Gonen PhD
UCLA, Los Angeles, ca, USA

10:55 - 11:15am
**370 48 or 370 to 1000 and More**
Lisa J. Keefe PhD
AUI - Center for Advancing Therapeutics, Lemont, IL, USA

11:15 - 11:30am
**195 In the Footsteps of Pasteur: Identifying Conglomerate Systems Using State-of-the-Art Electron Diffraction**
Gustavo Santiso-Quinones[1], Christian Jandl[1], Ivo B. Rietveld[2,3], Felix Painsecq[2], Gerard Coquerel[2], Laura Samperisi[1], Johannes Merkelbach[1], Gunther Steinfeld[1], Danny Stam[1]
[1]ELDICO Scientific AG, Allschwil, Basel Area, Switzerland. [2]Normandie University, Rouen, Normandy, France. [3]Université Paris Cité Cité, Paris, Paris, France

**1.1.4: Advances in Synchrotron-Based Characterization of Additive Manufacturing Processes & Properties**
8:30 - 11:30am Saturday, 19th July, 2025
Session Room: Lilac B
Chairs Hilmar Koerner, Arthur Woll
The session will delve into recent developments and importance of synchrotron x-ray scattering techniques in elucidating the development of intra- and inter-layer structures in materials during additive manufacturing (AM). Additive manufacturing technologies are proving to disrupt various industries by enabling the creation of complex, high-performance components with unparalleled design freedom. However, the current state of the art faces significant challenges, particularly in achieving consistent material properties and optimal performance. One of the critical hurdles is understanding the complex interplay between processing parameters, structural formation at various length scales, and the resulting performance properties of the manufactured parts. Synchrotron X-ray techniques (e.g. scattering, diffraction, imaging) offer a powerful means to monitor and analyze the real-time evolution of material structures at various length scales during the AM process. This session will highlight recent advancements, provide insights into overcoming existing challenges, and discuss how these techniques can drive the development of more reliable and high-performance additive manufacturing processes.

8:30 - 9:00am
**284 Investigating Additive Manufacturing Processes of Polymeric Materials with X-ray Scattering Techniques**
Dr. Lutz Wiegart PhD
National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA

9:00 - 9:30am
**258 Elucidating spatial heterogeneities in 3D printed thermoplastic elastomers using micro-beam small-angle x-ray scattering**
Alice S Fergerson, Emily C Davidson PhD

Princeton University, Princeton, NJ, USA

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9:30 - 10:00am

**312 Real-time Characterization of the Morphology of High-Performance Engineering Thermoplastics During Additive Manufacturing via Synchrotron X-ray Diffraction**

Dr. Kirt Page PhD[1,2,3], Jacob Crossno[1,2], Mia Carrola[2], Devin Ryan[1,2], Hilmar Koerner[2], Arthur Woll[3], Louisa Smieska[3]

[1]BlueHalo, Dayton, Ohio, USA. [2]Air Force Research Laboratory, Dayton, Ohio, USA. [3]Cornell High Energy Synchrotron Source, Ithaca, New York, USA

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10:30 - 11:00am

**279 Characterizing Residual Stresses in Additively Manufactured Alloys at the Cornell High Energy Synchrotron Source**

Kelly E Nygren PhD[1], Christopher Budrow PhD[2], Paul Shade PhD[3], Peter Ko PhD[1], Amlan Das PhD[1], Diwakar Naragani PhD[1], Arthur Woll PhD[1], Matthew P Miller PhD[1]

[1]Cornell University, Ithaca, New York, USA. [2]Budrow Consulting LLC, Albany, New York, USA. [3]Air Force Research Laboratory, Dayton, Ohio, USA

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11:00 - 11:30am

**322 Microstructure evolution in a precipitation-hardened high-entropy alloy fabricated by additive manufacturing**

Dr. Matthew J Luebbe[1], Dr. Fan Zhang[1], Dr. Haiming Wen[2]

[1]NIST, Gaithersburg, MD, USA. [2]Missouri University of Science and Technology, Rolla, MO, USA

### 1.1.5 General Interest I

8:30 - 11:30am Saturday, 19th July, 2025

Session Room: Lilac D

Chairs Tim Stachowski, 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

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8:30 - 9:00am

**32 The nitro-chloro substitution on two quinolinone-chalcones: from molecular modeling to antioxidant potential**

Ms Renata Layse G. de Paula Master[1], Dr Jean M.F. Custódio PhD[2], Dr Caridad Noda-Pérez PhD[3], Dr Allen G. Oliver PhD[2], Dr Hamilton B. Napolitano PhD[1,2]

[1]Universidade Estadual de Goiás, Anápolis, Goiás, Brazil. [2]University of Notre Dame, Notre Dame, Indiana, USA. [3]Universidade Federal de Goiás, Goiânia, Goiás, Brazil

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9:00 - 9:20am

**236 Static and Dymanic disorder in Formamidinium Lead Bromide Single Crystals**

Dr. Yael Diskin-Posner PhD

Weizmann Institute, Rehovot, Rehovot, Israel

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9:20 - 9:40am

**225 Five-Dimensional Positional Modulation with Quench-Trapped Modulation Phase in Solid-state Electrolyte Network Solid**

M. Brody Mistrot M.S., Dr. Michael J. Zdilla Ph.D.
Temple University, Philadelphia, PA, USA

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9:40 - 10:00am

**182 Uncovering the correlations between the structure and valence tautomerism in Co(Dioxolene)2Py2 crystals.**

Marcelo F. F. Alecrim M.Sc, Professor Carlos B. Pinheiro PhD, Professor Simone S. Alexandre PhD
Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, Minas Gerais, Brazil

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10:30 - 10:50am

**184 Data Archive Challenge: Transitioning Users to New IDs and Data File Format at the Protein Data Bank**

Brian P Hudson[1], Zukang Feng[1], Irina Persikova[1], Yuhe Liang[1], Ezra Peisach[1], Jasmine Y Young[1], wwPDB Team[1,2,3,4,5,6,7], Stephen K 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, -, United Kingdom. [3]PDBj, Institute for Protein Research, Osaka, -, Japan. [4]EMDB, EMBL-European Bioinformatics Institute, Hinxton, -, United Kingdom. [5]BMRB, UConn Health, Farmington, CT, USA. [6]PDBc, ShanghaiTech University and National Facility for Protein Science in Shanghai, Shanghai, -, China. [7]RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, San Diego, CA, USA

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10:50 - 11:10am

**196 Streamlining OneDep Depositions of Multiple Related 3DEM Entries with pdb_extract**

Dr. Justin W. Flatt Ph.D.[1], Dr. Chenghua Shao Ph.D.[1], Dr. Brian P. Hudson Ph.D.[1], Dr. Irina Persikova Ph.D.[1], Dr. Yuhe Liang Ph.D.[1], Dr. Zukang Feng Ph.D.[1], Dr. Ezra Peisach Ph.D.[1], Dr. Jasmine Young Ph.D.[1], wwPDB OneDep Team[1,2,3,4,5], Dr. Stephen K. Burley M.D., Ph.D.[1,6]
[1]RCSB Protein Data Bank, Rutgers, The State University of New Jersey, Piscataway, NJ, USA. [2]PDBe, EMBL-European Bioinformatics Institute, Hinxton, Cambridgeshire CB10 1SD, United Kingdom. [3]Institute for Protein Research, Osaka University, Suita, Osaka, Japan. [4]EMDB, EMBL-European Bioinformatics Institute, Hinxton, Cambridgeshire CB10 1SD, United Kingdom. [5]BMRB, UConn Health, Farmington, CT, USA. [6]RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, San Diego, CA, USA

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11:10 - 11:30am

**34 From single crystal neutron diffraction to single crystal diffraction imaging - amazing opportunities and developments**

Christina Hoffmann[1], James Martin[2], James Weng[3], Matthew Krogstad[4], Ella Schmidt[5], Reinhard Neder[6]
[1]ORNL, Oak Ridge, TN, USA. [2]NCSU, Raleigh, NC, USA. [3]BWXT, Lynchburg, VA, USA. [4]ANL, Argonne, IL, USA. [5]University of Bremen, Bremen, Lower Saxony, Germany. [6]Erlangen University, Erlangen, Bavaria, Germany

**PL1 Etter Award: Dr. Dmitry Lyumkis**
11:45am - 12:45pm Saturday, 19th July, 2025
Session Room: Junior Ballroom C
The ACA is proud to recognize Dr. Dmitry Lyumkis with the 2025 Margaret C. Etter Early Career Award for his groundbreaking contributions to structural biology and cryo-electron microscopy (cryo-EM). Dr. Lyumkis has advanced our understanding of infectious disease mechanisms, particularly HIV, through high-resolution structural insights into key viral protein complexes and their interactions with host cells.

A standout in both research and methodology, Dr. Lyumkis was among the first to resolve the structure of the HIV-1 envelope glycoprotein trimer, a pivotal breakthrough in vaccine development. His lab has since uncovered how viral intasomes integrate into host chromatin, how antiviral drugs block this process, and how resistance to therapy evolves. His innovations in cryo-EM, especially in overcoming sample preparation and validation challenges, have become widely adopted tools within the structural biology community.

Currently an Associate Professor at The Salk Institute and holder of the Hearst Foundations Chair, Dr. Lyumkis exemplifies the spirit of the Etter Award through his innovative science, leadership in the field, and profound impact on structural biology at large. We are honored to celebrate his achievements as a rising leader in the global scientific community.

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11:45am - 12:45pm
**346 Structural Basis of Activity of and Resistance to HIV Integrase Inhibitors**
Associate Professor Dmitry Lyumkis
Salk Institute for Biological Studies, La Jolla, CA, USA

**Three Minute Thesis**
12:45 - 1:45pm Saturday, 19th July, 2025
Session Room: Magnolia A
Chairs Alexander Erickson, Kenneth Childers
Join us for one of the most dynamic and engaging sessions of the conference—the Three Minute Thesis (3MT) competition! This fast-paced event challenges participants to present their research clearly and compellingly in just three minutes, using only one static slide. Whether you're competing or cheering from the audience, the 3MT is a great opportunity to discover cutting-edge work across the field, support your peers, and be inspired by the next generation of crystallographers. Don't miss it!

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**530 Hide and Go Seek: Finding the Locations of Ca, Zn, and S ions within LTA Zeolite Modified for $H_2S$ Capture**
Adeyemi D Ojaide, Dr Stacey J Smith Doctorate, Dr Roger G Harrison Doctorate
Brigham Young University, Provo, UT, USA

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**532 The structural basis for synergistic inhibition of geranylgeranyl diphosphate synthase with stereoisomeric triazole bisphosphonates**
Andrew Pham, Sarah Holstein, Gloria Borgstahl
UNMC, Omaha, NE, USA

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**533 Non-Averaged Single-Molecule 3D Structures Capture RNA Maturation Intermediates by Individual-Particle Cryo-Electron Tomography**

Dr. Gang Ren PhD, Dr. Jianfang Liu PhD, Dr. Meng Xhang
LBNL, Berkeley, CA, USA

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**534 Low-Temperature Synthesis and Characterization of Hybrid Heavy Metal Zero-Dimensional Cluster Compounds Containing Pt/Ir and Bi.**
Gayomi Kanchana Samarakoon Mudiyanselage BSc, Logan Schilling, Professor Sviatoslav Baranets PhD
Louisiana State Univesity, Baton Rouge, LA, USA

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**535 New Methods in RNA Structural Biology: TELSAM Protein Chaperone Crystallography Applications to Folded RNA**
Jacob C Averett, Miles Bradford, Blake Averett, Dalton Hansen, Dr. James D Moody
Brigham University, Provo, UT, USA

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**536 Uncovering the correlations between the structure and valence tautomerism in Co(Dioxolene)2Py2 crystals.**
Marcelo F Alecrim MSc[1], Carlos B Pinheiro[2], Simon S Alexandre PhD[1]
[1]Universidade Federal de Minas Gerais (UFMG), Belo Horizonte,, Minas, Gerais, Brazil.
[2]Universidade Federal de Minas Gerais (UFMG), Belo Horizonte,, Minas Gerais, Gerais, Brazil

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**537 Structural and Functional Characterization of SOSTDC1**
Melissa Gouge B.S, Gregory Gibson, Chandramohan Kattamuri PhD, Thomas B Thompson
University of Cincinnati, Cincinnati, OH, USA

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**538 Using Neutrons to Elucidate the Catalytic Shift from Superoxide Dismutase to Peroxidase Activity in Fe-Substituted Human MnSOD**
Miles Graham B.S, Dr. Gloria E.O. Borgstahl PhD
University of Nebraska Medical Center, Omaha, NE, USA

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**539 Antagonist development for the CMG2 protein**
Ms Prasadika Samarawickrama Hetti Arachchige PhD, Ms Fang Fang, Dr James Moody, Dr Ken Christensen
Brigham Young University, Provo, UT, USA

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**541 Dual Substrate Binding stabilizes the Catalytic State in Ketohexokinase**
So Young Bae PhD, Karen Allen, Dean R Tolan
Boston University, Boston, MA, USA

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**542 STARS: Creating robust infrastructure to scale up structural biology programs for students**
Susanna Huang
Georgia Institute of Technology, Atlanta, GA, USA

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**543 De novo ß-hairpin design using a residue-based physicochemical property landscape**
Dr Vardhan Satalkar phD, Prof. Julie Mitchell, Prof. Matthew Torres

Georgia Institute of Technology, Atlanta, GA, USA

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**544 A pH-Triggered TELSAM Approach for Rapid, Tag-Free Protein Purification and Crystallization**

Wisdom Oshireku Abiodun, Celeste Litchfield, Mikaela Burtch, Jamison Cartwright, James D Moody
Brigham Young University, Provo, UT, USA

**TR2: Transactions II Evolving Landscape of Structural Science: AI and Multimethod Approaches**

2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Junior Ballroom C
Chairs Thomas Proffen, George Lountos, Krystle McLaughlin, Carla Slebodnick

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2:00 - 2:30pm

**146 PDB-IHM: A System for Archiving and Dissemination of integrative structures**

Dr Brinda Vallat Ph.D.
RCSB PDB, Rutgers University, Piscataway, NJ, USA

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2:30 - 3:00pm

**152 Non-Averaged Single-Molecule 3D Structures Capture RNA Maturation Intermediates by Individual-Particle Cryo-Electron Tomography**

Dr. Gang Ren PhD, Dr. Jianfang Liu PhD, Dr. Meng Zhang PhD
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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3:30 - 4:00pm

**200 Structural Biology-Guided Multiomics of the Human Microbiome**

Professor Mattthew R. Redinbo PhD
University of North Carolina, Chapel Hill, NC, USA

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4:00 - 4:30pm

**285 The 7th Blind Test of CSP Methods: Triumphs, Challenges and Insights**

Dr. Susan M Reutzel-Edens PhD[1], Dr. Lily M Hunnisett PhD[2]
[1]SuRE Pharma Consulting, LLC, Zionsville, IN, USA. [2]Cambridge Crystallographic Data Centre, Cambridge, CB2 1EZ, United Kingdom

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4:30 - 5:00pm

**75 Accelerating Synchrotron MX Beamlines: Automated Sample Centering with Machine Learning and Bluesky Orchestration**

David Aragao PhD[1], Martin Savko[2], Dominic Oram[1], Kate Smith[3], William Shepard[2], Ralf Flaig[1]
[1]Diamond Light Source, Didcot, Oxforshire, United Kingdom. [2]Synchrotron SOLEIL, Gif-sur-Yvette, NA, France. [3]Australian Synchrotron, Australian Nuclear Science and Technology Organisation, Clayton, Victoria, Australia

**1.2.1 Neutrons in Structural Biology**

2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Lilac D

Chairs Gloria Borgstahl, Duminda Liurukara

Neutron scattering is a powerful tool to study the structure-function relationship of biomacromolecules and biomolecular complexes. Neutrons display a distinct sensitivity to the positions and motions of hydrogen atoms, the most abundant and elusive element found in biological systems, able to provide unique, complementary information to that gained from traditional structural biology techniques. Some capabilities of neutron scattering methods include that ability to locate individual hydrogen positions with atomic resolution, structural analysis of large-scale assemblies, and dynamics ranging from femto- to microsecond time scales. This session aims to highlight the exciting research benefiting from neutron-based structural techniques and bring attention to the advantages of using neutrons in structural biology.

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2:00 - 2:30pm

**424 Unraveling protein catalysis through neutron diffraction**

Dean A. Myles

Oak Ridge National Laboratory, Oak Ridge, TN, USA

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2:30 - 3:00pm

**427 Interrogating Low Barrier Hydrogen Bonds with Neutrons, X-rays, and Computation**

Jiusheng Lin[1], Oksana Gerlits[2], Daniel W. Kneller[3], Kevin L. Weiss[3], Leighton Coates[3], Mark A. Hix[4], Solomon Y. Effah[4], Andrey Kovalevsky[3], Alice R. Walker[4], Mark A. Wilson[5]

[1]University of Nebraska, Lincoln, NE, Taiwan. [2]Tennessee Wesleyan University, Athens, TN, USA. [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [4]Wayne State University, Detroit, MI, USA. [5]University of Nebraska, Lincoln, NE, USA

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3:30 - 4:00pm

**106 Neutrons & MnSOD: Past & Future**

Dr. Medhanjali Dasgupta Ph.D, Dr. Gloria Borgstahl

University of Nebraska Medical Center, Omaha, NE, USA

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4:00 - 4:15pm

**162 Using Neutrons to Elucidate the Catalytic Shift from Superoxide Dismutase to Peroxidase Activity in Fe-Substituted Human MnSOD**

Miles Graham B.S., Dr. Gloria E. O. Borgstahl Ph.D

University of Nebraska Medical Center, Omaha, NE, USA

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4:15 - 4:40pm

**202 Unraveling Unique Effect of Ergosterol on Lipid Membranes, and What We Can Do with the Future STS**

Shuo Qian Ph.D., Gergely Nagy, Piotr Zolnierczuk, Eugene Mamontov, Robert Standaert

Oak Ridge National Laboratory, Oak Ridge, TN, USA

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4:40 - 5:00pm

**259 Probing SARS-CoV-2 Nsp8 Condensates with Neutron Scattering**

Sharique Khan[1], Wellinton Leite[1], Brighton Miller[2], Hugh O'Neill[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]University of Notre Dame, Notre Dame, IN, USA

**1.2.2 MicroED for Small Molecules**
2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Magnolia A
Chairs Fernando Castro, Joseph Ferrara
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.

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2:00 - 2:20pm
**174 Electron Diffraction (Micro-ED): A dedicated device and its applications in the pharmaceutical industry**
Dr Gustavo Santiso-Q Ph.D., Dr. Christian Jandl, Dr. Johannes Merkelbach, Dr. Laura Samperisi, Dr. Gunther Steinfeld s, Danny Stam
Eldico Scientific, Allschwil, Basel-Landschaft, Switzerland

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2:20 - 2:40pm
**235 Mega-electron-volt Microcrystal Electron Diffraction**
Dr. Xiaozhe Shen Ph.D.[1], Dr. Duan Luo Ph.D.[2], Prof. Xijie Wang Ph.D.[3,4]
[1]Institute of Advanced Science Facilities, Shenzhen, Guangdong, China. [2]Key Laboratory of Ultrafast Photoelectric Diagnostics Technology, Xi'an Institute of Optics and Precision Mechanics, Chinese Academy of Sciences, Xi'an, Shaanxi, China. [3]University of Duisburg-Essen, Duisburg, North Rhine-Westphalia, Germany. [4]TU Dortmund University, Dortmund, North Rhine-Westphalia, Germany

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2:40 - 3:00pm
**189 High-Throughput, Automated Molecular Replacement for Small Molecule MicroED Data**
Adam Thibodeaux, Emma Rova-Danelius
University of California Riverside, Riverside, CA, USA

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3:30 - 3:50pm
**91 The Transformative Effect of Electron Diffraction**
Dr. Pierre Le Magueres Ph.D.[1], Dr. Joseph D Ferrara Ph.D.[1], Dr. Robert Bücker Ph.D.[2]
[1]Rigaku Americas, The Woodlands, TX, USA. [2]Rigaku europe SE, Neu-Isenburg, Hesse, Germany

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3:50 - 4:10pm
**311 Using Electron Diffraction and Diffuse Scattering to Investigate the Vacancy Network of Prussian Blue**
Gabriella N. Ruiz, Serhii Vasylevskyi, Michael J. Rose
The University of Texas at Austin, Austin, TX, USA

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4:10 - 4:30pm
**385 Microcrystal electron diffraction-guided discovery of natural products**

David A Delgadillo PhD
California Institute of Technology, Pasadena, CA, USA

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4:30 - 5:00pm
**344 microED/3DED in a Shared Facility: Optimizing the pipeline**
Professor Chris D. Malliakas PhD
Northwestern University, Evanston, IL, USA

**1.2.3 Utilizing in Situ and Operando Techniques to Elucidate Complex Systems**
2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Magnolia BC
Chairs Saul Lapidus, Cheng Li
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.

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2:00 - 2:20pm
**89 The formation, phase behavior and properties of helium fluoroperovskites as seen by in-situ X-ray and neutron powder diffraction**
Angus P Wilkinson[1], Shangye Ma[1], Jamie Molaison[2], Antonio dos Santos[2]
[1]Georgia Institute of Technology, Atlanta, GA, USA. [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA

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2:20 - 2:40pm
**191 Pressure-Induced Structural Evolution and Negative Compressibility in Hybrid Metal Oxides**
Raúl Torres-Cadena[1], W. Lakna N. Dayaratne[1], Hsing-Ta Chen[1], Evgenii L. Kovrigin[1], Matthew G. Tucker[2], Bianca Haberl[2], Adam Jaffe[1]
[1]University of Notre Dame, Notre Dame, IN, USA. [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA

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2:40 - 3:00pm
**204 Autonomous Reduction and Analysis of 2D Diffraction and Scattering Data**
Anna H Merritt PhD, Wenqian Xu, Olaf Borkiewicz, Miaoqi Chu, Nicholas Schwarz, Brian Toby, James Weng
Argonne National Laboratory, Lemont, IL, USA

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3:30 - 3:55pm

**178 Structure-property relationships of emerging adsorbents as resolved via in-situ powder diffraction and other techniques**
Hayden Evans
NIST, Gaithersburg, MD, USA

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3:55 - 4:15pm
**345 Neutron scattering studies of porous material**
CHENG LI
ORNL, Oak Ridge, TN, USA

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4:15 - 4:35pm
**323 Microstrain screening towards defect-less layered transition metal oxide cathodes**
Dr. Tianyi Li Ph.D.
Argonne National Laboratory, Lemont, IL, USA

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4:35 - 5:00pm
**170 Revealing Reaction Mechanisms and Enabling Materials Discovery in Fluxes through Panoramic Synthesis**
Xiuquan Zhou Ph.D[1], Hengdi Zhao Ph.D[2], Mercouri G Kanatzidis Ph.D[3]
[1]Georgetown University, Washington, DC, USA. [2]Argonne National Laboratory, Lemont, IL, USA. [3]Northwestern University, Evanston, IL, USA

**1.2.4 Crystallographic Data Analysis and Processing**
2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Lilac B
Chairs Aaron Brewster, Dominika Borek
This session focuses on methodologies and innovative techniques in the analysis and processing of crystallographic data. We are seeking contributions that present novel algorithms, software tools, and workflows that enhance the accuracy, efficiency, and robustness of data analysis in crystallography. Abstracts should cover topics such as data collection optimization, error reduction strategies, and data integration.

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2:00 - 2:20pm
**165 Robust error calibration for serial crystallography**
David W. Mittan-Moreau, Vanesa Oklejas, Daniel W. Paley, Asmit Bhowmick, Jan Kern, Nicholas K. Sauter, Aaron S. Brewster
Lawrence Berkeley National Lab, Berkeley, CA, USA

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2:20 - 2:40pm
**210 Abismal: Approximate Bayesian Inference for Scaling and Merging at Advanced Lightsources**
Doris Mai[1], Doeke R Hekstra[2], Frédéric Poitevin[1], Kevin M Dalton[1,3]
[1]Machine Learning and Computer Vision Group, LCLS Data Systems, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [2]Department of Molecular & Cellular Biology, Harvard University, Cambridge, MA, USA. [3]Department of Biology, New York University, New York, NY, USA

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2:40 - 3:00pm
**329 Memory and Algorithmic Constraints of GPUs in Diffraction Data Processing**
Zbyszek Otwinowski Ph.D.[1], Raquel Bromberg Ph.D.[2,1]
[1]UT Southwestern Medical Center, Dallas, TX, USA. [2]Ligo Analytics, Dallas, TX, USA

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3:30 - 3:48pm
**98 Quantifying Pseudosymmetry in Molecular Crystals**
Prof. Inbal Tuvi-Arad
The Open University of Israel, Raanana, Israel, Israel

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3:48 - 4:06pm
**11 I bnl compress: Lossy but not lossy compression, a python script to compress MX data**
Dr. Herbert J Bernstein PhD[1], Dr. Jean Jakoncic PhD[2]
[1]Fresh Pond Research Institute, Cambridge, MA, USA. [2]Brookhaven National Laboratory, Upton, NY, USA

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4:06 - 4:24pm
**211 Fast-feedback for unattended data collection at Diamond Light Source**
Dr Nicholas Devenish, Dr James Beilsten-Edmands, Mr Dimitrios Vlachos
Diamond Light Source, Didcot, Oxfordshire, United Kingdom

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4:24 - 4:42pm
**318 Automated Data Merging, Analysis and Structure Solution in RAPD2**
Dr. Kay Perry PhD[1,2], Dr. Frank V Murphy PhD[1,2], Dr. David Neau PhD[1,2], Dr. Jonathan Schuermann PhD[1,3]
[1]Cornell University, Ithaca, NY, USA. [2]Northeastern Collaborative Access Team, Lemont, IL, USA. [3]Northeastern Collaborative Access Team, Lemont, NY, USA

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4:42 - 5:00pm
**338 Integrated Platform for Assessing the Quality of Macromolecular Models**
Wojciech Dec[1,2,3], Pawel Rubach Ph.D.[4,1], Wladek Minor Ph.D.[1]
[1]Department of Molecular Physiology and Biological Physics University of Virginia, School of Medicine, Charlottesville, Virginia, USA. [2]Department of Computational Biophysics and Bioinformatics, Jagiellonian University, Krakow, Malopolska, Poland. [3]Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Malopolska, Poland. [4]Warsaw School of Economics, Warsaw, Mazowieckie, Poland

**1.2.5 Innovations in Sample Preparation and other Hardware in CryoEM**
2:00 - 5:00pm Saturday, 19th July, 2025
Session Room: Lilac AC
Chairs David Taylor, Edward Eng
Developments in cryoEM and cryoET methods and technology have revolutionized our ability to see the atomic structure of proteins and biological macromolecules in the cellular environment. In this session, we explore and discuss new developments in sample preparation and EM technologies that address current challenges and open doors to exciting areas of biology.

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2:00 - 2:30pm

**37 Advances in Microsecond Time-Resolved Cryo-EM**

Ulrich J. Lorenz

EPFL, Lausanne, VD, Switzerland

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2:20 - 2:40pm

**26 Native mass spectrometry prescreening of G protein-coupled receptor complexes for cryo-EM structure determination**

Donggyun Kim PhD[1], Weijing Liu PhD[2], Prof. Vadim Cherezov PhD[1], Rosa I Viner PhD[2]

[1]University of Southern California, Los Angeles, CA, USA. [2]Thermo Fisher Scientific, San Jose, CA, USA

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2:40 - 3:00pm

**341 Apollo: An Event-Based Direct Detector for MicroED**

Michael S Spilman Ph.D.

Direct Electron LP, San Diego, CA, USA

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3:30 - 3:55pm

**52 Expanding the Toolkit for Structural Cell Biology with ExoSloNano**

Lindsey N Young PhD[1], Alice Sherrard PhD[2], Huabin Zhou PhD[3], Farhaz Shaikh[4], Joshua Hutchings PhD[5], Margo Riggi PhD[6], Mythreyi Narasimhan PhD[1], Eric Bennett PhD[1], Michael Rosen PhD[3,7], Antonio Giraldez PhD[2], Elizabeth Villa PhD[1,8]

[1]UCSD, La Jolla, CA, USA. [2]Yale University, New Haven, CT, USA. [3]UT Southwestern, Dallas, TX, USA. [4]UCSF, San Francisco, CA, USA. [5]Chan Zuckerberg, Redwood City, CA, USA. [6]MPI, Munich, Bavaria, Germany. [7]HHMI, Dallas, TX, USA. [8]HHMI, La Jolla, CA, USA

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3:55 - 4:15pm

**185 A 2.8-Å resolution structure of the skatole-producing glycyl radical enzyme Indoleacetate Decarboxylase enabled by new techniques in cryo-EM grid preparation.**

Christa N Imrich, Dr. Lindsey RF Backman PhD, Dr. Mary C Andorfer PhD, Prof. Catherine L Drennan PhD

Massachusetts Institute of Technology, Cambridge, MA, USA

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4:15 - 4:35pm

**172 MagIC-Cryo-EM: Structural determination on magnetic beads for scarce macromolecules in heterogeneous samples**

Assistant Professor Yasuhiro Arimura Ph. D.

Fred Hutchinson Cancer Center, Seattle, WA, USA

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4:35 - 5:00pm

**63 Small LEA proteins mitigate air-water interface damage to fragile cryo-EM samples during plunge freezing**

Kaitlyn M Abe[1], Gan Li[1,2], Qixiang He[1], Assistant Professor Timothy Grant Ph.D.[1,2], Assistant Professor Ci Ji Lim Ph.D.[1]

[1]University of Wisconsin-Madison, Madison, WI, USA. [2]Morgridge Institute for Research, Madison, WI, USA

**PS1: Poster Session #1**
5:30 - 7:30pm Saturday, 19th July, 2025
Session Room: Exhibit Hall
Chairs Tim Stachowski, Leighanne Gallington, Cora Lind-Kovacs
Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don't miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

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**433 Active Site Loop Dynamics of PriB, a C-prenyltransferase**
Omowumi Oreoluwa Fagbohun M.Sc., Dr. Jonathan Clinger Ph.D.
Baylor University, Waco, Texas, USA

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**461 A pH-Triggered TELSAM Approach for Rapid, Tag-Free Protein Purification and Crystallization**
Wisdom Oshireku Abiodun, Celeste Litchfield, Mikaela Burtch, Jamison Cartwright, James D Moody
Brigham Young University, Provo, Utah, USA

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**33 Cyclization Effects of Methoxy-Chalcones on Oxidative Stability: Impact on Biodiesel Additives**
Dr Vitor Santos Duarte PhD[1], Dr Hamilton Barbosa Napolitano PhD[1], Dr Pal Perjesi PhD[2]
[1]Universidade Estadual de Goiás, Anápolis, Goiás, Brazil. [2]University of Pécs, Pécs, Baranya, Hungary

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**66 The Additive Game: investigating methods to stabilize thin-layer cryo-EM specimens**
Mahitha Roy M.S., Dominika Borek PhD, Zbyszek Otwinowski PhD
University of Texas Southwestern Medical Center, Dallas, TX, USA

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**214 Visualizing Oxysterol-binding Protein Ligand-Triggered Structural Signals**
Walter Galie[1], Ruth Fiona Bayimenye[2], Dr. Anthony Burgett[2], Dr. Christina Bourne[1]
[1]The University of Oklahoma, Norman, OK, USA. [2]The University of Oklahoma Health Sciences, Oklahoma City, OK, USA

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**298 Structural insights into state transition and end-processing in non-homologous end joining from cryo-EM**
Alex Vogt[1], Yuan He[2]
[1]Northwestern University, Evanston, IL, USA. [2]Johns Hopkins University, Baltimore, MD, USA

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**315 Automated high-throughput high-resolution X-ray diffraction capabilities at SSRL BL 2-1**
Dr Sikhumbuzo Masina, Dr Monty Cosby, Dr Nicholas Strange, Dr Vivek Thampy, Mr Charles Troxel Jr, Dr Kevin Stone
SLAC/SSRL, Menlo Park, CA, USA

**325 Structural insights into a high-fidelity CRISPR-Cas12a variant revealed using optimized graphene oxide cryo-EM grids**

Chhandosee Ganguly, Dr. Swarmistha Aribam, Dr. Leonard M. Thomas, Dr. Rakhi Rajan
Department of Chemistry and Biochemistry, Price Family Foundation Institute of Structural Biology, Stephenson Life Sciences Research Center, University of Oklahoma, Norman, Oklahoma, USA

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**436 Structural diversity and polymorphism in amyloid fibrils from single organs and single patients with AL amyloidosis**

Parker T Bassett BS[1], Dr. Lorena Saelices PhD[1], Dr. Binh Nguyen PhD[1], Dr. Virender Singh PhD[1], Dr. Gareth Morgan PhD[2]
[1]UT Southwestern Medical Center, Dallas, TX, USA. [2]Boston University, Boston, MA, USA

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**441 *De novo* ß-hairpin design using a residue-basedphysicochemical property landscape**

Dr. Vardhan Satalkar Ph.D[1], Prof. Julie Mitchell[2], Prof. Mathhew Torres[1]
[1]Georgia Institute of Technology, Atlanta, Georgia, USA. [2]University of Wisconsin, Maddison, Wisconsin, USA

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**450 Covalent Organic Frameworks: A 2D Platform for Controlled Nanostructuring of Single Ion Magnets**

Noreen Mazhar Graduate Student, Dr. Mario Wriedt Professor (PI)
The University of Texas at Dallas (UTD), Dallas, Texas, USA

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**452 Metal-Organic Frameworks: NU-1000 a Sensing Probe for the Detection of Water Contaminants**

Nafees Iqbal Graduate Student, Dr. Mario Wriedt Professor (PI)
The University of Texas at Dallas (UTD), Dallas, Texas, USA

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**403 Solution Characterization and Initial Crystallization Studies of ΔTrbB from the F Plasmi**

Maya Soko, Gerald Audette
York University, Toronto, Ontario, Canada

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**438 Structural Determination of the Interaction of $H_2S$ and Insulin**

Christina S Rodriguez, Ming Fu, Dr. Rui Wang, Dr Gerald F Audette
York University, Toronto, ON, Canada

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**418 Structural and functional insights into *Escherichia coli* O32:H37 contact dependent inhibition**

Karolina Michalska[1,2], Lucy Stols[1], Dinh Quan Nhan[3], Fernando Garza-Sánchez[3], William H. Eschenfeldt[1], Christopher S. Hayes[3,4], Andrzej Joachimiak[1,2,5]
[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL, USA. [2]Center for Structural Biology of Infectious Diseases, Consortium for Advanced Science and Engineering, University of Chicago, Chicago, IL, USA. [3]Department of Molecular, Cellular and Developmental Biology, University of California, Santa Barbara, CA, USA. [4]Biomolecular Science and Engineering

Program, University of California, Santa Barbara, CA, USA. [5]Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL, USA

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**428 Structural Science and Disabilities**
Assoc. Prof. Andrew J Howard PhD
Illinois Institute of Technology, Chicago, IL, USA

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**431 *The Crucial Role of Water Molecules in Stabilizing the Repressor/Operator Complex in the TrpR Repressor Family***
Andrzej Joachimiak PhD[1,2], Youngchang Kim PhD[2], Natalia Maltseva PhD[1]
[1]University of Chicago, Chicago, IL, USA. [2]Argonne National Laboratory, Lemont, IL, USA

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**432 X-ray crystal structures *Corynebacterium diphtheriae* sortases**
Jerzy Osipiuk[1,2], Poonam Kamari[3], HyLam Ton-That[4], Hung Ton-That[3], Andrzej Joachimiak[1,5]
[1]Argonne National Laboratory, Lemont, IL, USA. [2]University of CHicago, Chicago, IL, USA. [3]University of California Los Angeles, Los Angeles, CA, USA. [4]University of California, Irvine, CA, USA. [5]University of Chicago, Chicago, IL, USA

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**440 Advancing Crystallography Research: The Latest Progress and Future Directions of NE-CAT Beamlines at the Advanced Photon Source**
Ali Kaya, Malcolm Capel, Igor Kourinov, Anthony Lynch, Anne Mulichak, David Neau, Kay Perry, Cyndi Salbego, Jonathan Schuermann, Narayanasami Sukumar, Graeme Winter, James Withrow, Frank Murphy
Cornell University, Lemont, IL, USA

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**16 Crystallography at CCSU- Twenty years of teaching crystallography to undergraduates at a small regional undergraduate institution.**
Dr Guy Crundwell PhD; Chemistry
CCSU, New Britain, CT, USA

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**28 Crystal Structures of Large-Volume Commercial Pharmaceuticals**
James A Kaduk PhD[1], Anja Dosen PhD[2], Thomas N Blanton PhD[2]
[1]North Central College, Naperville, IL, USA. [2]ICDD, Newtown Square, PA, USA

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**197 Small-Angle Neutron Scattering Instrument Concepts for Second Target Station of SNS**
Shuo Qian Ph.D.
Oak Ridge National Laboratory, Oak Ridge, TN, USA

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**463 Accelerating discovery and rational engineering of antibody modalities using Cryo-EM**
Dr. Tilak Gupta, Dr. Surajit Banerjee
Thermo Fisher Scientific, Portland, Oregon, USA

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**464 A high-throughput, rapid mail-in program for XFEL chemical crystallography at the Linac Coherent Light Source**

Dr Elyse A. Schriber PhD[1], Dr Daniel J. Rosenberg PhD[1], Dr. Daniel W. Paley PhD[2], Dr. Frederic Poitevin PhD[1], Maggie C. Willson[3], Kelsey Banta[1], Prof J. Nathan Hohman PhD[3], Dr. Aaron Brewster PhD[2]
[1]SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [3]University of Connecticut, Storrs, CT, USA

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**480 Understanding autism: structural and functional characterization of PTCHD1**
Professor Adrian Goldman Ph.D.[1], Ms Mimmu K Hiltunen M.Sc.[1], Dr. Orquidea Ribeiro Ph.D.[1], Professor Natalia Riobo-del Galdo PhD[2]
[1]University of Helsinki, Helsinki, Uusimaa, Finland. [2]University of Leeds, Leeds, West Yorkshire, United Kingdom

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**449 Cationic Covalent Organic Framework as Fluorescent Sensor for the Detection of Poly- and Perfluoroalkyl Substances (PFAS)**
Ms Maryam Piroozzadeh
university of texas at dallas, richardson, texas, USA

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**498 The Reciprocal Space Station Forum for Structural Scientists**
Doris Mai[1], Kara A Zielinski[2], Kevin M Dalton[1]
[1]Machine Learning and Computer Vision Group, LCLS Data Systems, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. [2]School of Applied and Engineering Physics, Cornell University, Ithaca, NY, USA

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**503 Structural Basis of Human Astrovirus Entry via FcRn and Antibody Neutralization**
Sashank Agrawal PhD, Ian A Wilson PhD
The Scripps Research Institute, La Jolla, California, USA

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**504 Studies on Radiation Damage to Improve the Efficiency and Data Quality**
Palani Kandavelu Ph.D, Zhongmin Jin Ph.D, , Zheng-Qing "Albert" Fu Ph.D, John Chrzas Ph.D, John P. Rose, Bi-Cheng Wang Ph.D
SER-CAT/University of Georgia, Athens, GA, USA

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**501 Structural Insights into Broadly Reactive SARS-CoV-2 Antibodies for Vaccine Design**
Morgan E Abernathy Ph.D., Christopher O Barnes Ph.D.
Stanford University, Stanford, CA, USA

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**502 Exploring PPM1D Phosphatase Structure for Next-Generation Small Molecule Inhibitor Development**
Jay P. Kumar[1], Dalibor Kosek[2,3], Stewart Durell[1], Nadya I. Tarasova[4], Lisa Jenkins[1], Subrata Debnath[1], Nathan Coussens[5], Matthew Hall[5], Daniel Appella[2], Fred Dyda[2], Sharlyn Mazur[1], Ettore Appella[1]
[1]National Cancer Institute, NIH, Bethesda, MD, USA. [2]NIDDK, National Institutes of Health, Bethesda, MD, USA. [3]Institute of Physiology of the Czech Academy of Sciences, Vestec, Prague, Czech Republic. [4]National Cancer Institute, NIH, Frederick, MD, USA. [5]National Center for Advancing Translational Sciences, NIH, Rockville, MD, USA

**483 Topobexin Targets a Unique Druggable Pocket of Topoisomerase II for Beta Isoform-Selective Control of DNA Damage During Anthracycline Chemotherapy**

Jan Kubes[1], Galina Karabanovich[1], Anh T.Q. Cong[2], Iuliia Melnikova[1], Olga Lencova[1], Petra Kollarova[1], Hana Bavlovic Piskackova[1], Veronika Kerestes[1], Lenka Applova[1], Lise C.M. Arrouye[2], Julia R. Alvey[2], Jasmina Paluncic[2], Taylor L. Witter[2], Anna Jirkovska[1], Jiri Kunes[1], Petra Sterbova-Kovarikova[3], Caroline A. Austin[4], Martin Sterba[1], Tomas Simunek[1], Jaroslav Roh[1], Matthew J. Schellenberg[2]

[1]Charles University, Hradec Kralove, HK, Czech Republic. [2]Mayo Clinic, Rochester, MN, USA. [3]Charles University, Rochester, HK, Czech Republic. [4]Newcasle University, Newcastle Upon Tyne, UK, United Kingdom

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**489 Lithium Coordination Complexes and Polymers of 1,4-Diazines**

George D Tisdale, Fahmida Islam M.S., Assistant Professor Clifton L Wagner Ph.D.
Louisiana State University, Baton Rouge, LA, USA

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**491 Decoding electromechanical coupling in shaker potassium ion channel: Intermediate voltage sensor and close pore**

Dr. Richa Agrawal PhD, Mr. Ramon Mendoza Uriarte, Dr. Bernardo Pinto PhD, Dr. Trayder Thomas PhD, Dr. Francisco Bezanilla PhD, Dr. Eduardo Perozo PhD, Dr. Benoit Roux PhD
Department of Biochemistry and Molecular biology, University of Chicago,, Chicago, IL, USA

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**522 Structural Insights into Escherichia coli Fructose-1-Phosphate Kinase Reveal Evolutionary Divergence within the PfkB Family**

Soyoung Bae PhD, Katie M Satko PhD, Dean R Tolan PhD
Boston University, Boston, MA, USA

**YSIG Mixer**

8:00 - 10:00pm Saturday, 19th July, 2025
Session Room: Offsite: Millers Ale House

Join us on Saturday, July 19th at 8:00 PM CDT at Miller's Ale House (70 Yorktown Shopping Center, Lombard, IL 60148)—just a short distance from the hotel.
You're welcome to make your own way there, or hop on one of our **complimentary shuttles** departing from the front of The Westin Lombard Chicago at **7:45 PM, 8:00 PM,** and **8:15 PM CDT**. Return shuttles will leave Miller's Ale House at **9:45 PM, 10:00 PM,** and **10:15 PM CDT**.

Each guest will receive one drink ticket, with a cash bar available for additional beverages. We'll also be serving a selection of appetizers, including boneless wings, mini cheeseburgers, mozzarella sticks, fried potstickers, spinach artichoke dip, and gluten-free options. Please note: food will be served, but it is not intended to replace a full meal.

This is one of the most anticipated social events of the conference—don't miss the chance to connect with new and familiar colleagues in a fun, relaxed setting.

As always, please drink responsibly and make choices that ensure a safe and enjoyable evening for all.

**Registration Desk**
7:30am - 5:00pm Sunday, 20th July, 2025
Session Room: Grand Ballroom Foyer

**Speaker Ready Room**
7:30am - 5:00pm Sunday, 20th July, 2025
Session Room: Walnut

**2.1.1 Emerging Modalities for Pharma Part 1**
8:30 - 11:30am Sunday, 20th July, 2025
Session Room: Junior Ballroom C
Chairs Elizabeth Sprague, Susmith Mukund
This session will focus on the application of cryo-EM, x-ray crystallography and complementary biophysical and computational methods to the discovery and optimization of various drug modalities. For decades, small molecules by far have been the preferred modality to tackle diseases. While the past couple of decades have seen an exciting influx of transformative therapeutic antibodies, today, several other "non-standard" entities such as PROTACs, antibody-like scaffolds, macrocycles, peptides, covalent modulators, to name a few, are being developed to address unmet medical needs. We welcome submissions showcasing relevant structural biology techniques to drug discovery.

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8:41 - 9:05am
**404 Structural biology in discovery and development of heterobifunctional degraders**
Associate Director Kunhua Li Ph.D.
Kymera Therapeutics, Watertown, MA, USA

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9:06 - 9:20am
**27 Rapid PROTAC discovery, design and testing by coupling crystallography and biology**
Debanu Das Ph.D.[1,2], Thomas Pesnot Ph.D.[3]
[1]Accelero Biostructures, San Carlos, CA, USA. [2]XPose Therapeutics, San Carlos, CA, USA.
[3]Concept Life Sciences, Chapel-en-le-Frith, High Peak, United Kingdom

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9:21 - 9:35am
**31 Structural Insights into PROTAC Complex Formation from Analytical Ultracentrifugation and Hydrodynamic Modeling**
Alexander E Yarawsky PhD, Lake N Paul PhD
BioAnalysis, LLC, Philadelphia, Pennsylvania, USA

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9:36 - 10:00am
**252 Structural Insights into HPV16 E6:E6AP:p53 Complex Formation and Inhibition by Covalent Peptides**
Dr. Aaron H Nile PhD
Calico Life Sciences LLC, South San Francisco, CA, USA

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10:30 - 10:50am
**45 Cryo-EM structure of the TL1A-DR3 complex and implications for the treatment of Inflammatory Bowel Disease**

Cameron L Noland PhD, Marcelo Murai, Paulo Zaragoza, Ben Bell, Sultan Yilmaz, Shruti Nayak, Esme Alarcon, Michael Eddins, Todd Mayhood, Yunpeng Zhou, Burt Barnett, Haihong Zhou, Johan Fransson
Merck & Co., Inc., Rahway, NJ, USA

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10:51 - 11:10am
**61 Mechanism of Herpes Simplex Virus Inhibition by Antiviral Compounds**
Dr Qing Yao Ph.D.
Gilead Sciences, Inc., Foster City, CA, USA

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11:11 - 11:30am
**134 Enabling HighThroughput Electron Cryo-microscopy for Drug Discovery**
Dr Pamela A Williams
Astex Pharmaceuticals, Cambridge, Cambs, United Kingdom

### 2.1.2 Hot Structures

8:30 - 11:30am Sunday, 20th July, 2025
Session Room: Magnolia A
Chairs James Moody, Chhandosee Ganguly, George Lountos
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, CryoEM, Small Angle X-ray Scattering, or hybrid methods including those that incorporate predictive / computational modeling.

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8:30 - 8:50am
**5 Fast hit generation for discovery of inhibitors of DNA repair protein Pol eta**
Debanu Das
XPose Therapeutics, San Carlos, CA, USA. Accelero Biostructures, San Carlos, CA, USA

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8:50 - 9:10am
**379 Naturally ornate RNA homo-oligomeric complexes**
Rachael Kretsch[1], Yuan Wu[1], Svetlana A Shabalina[2], Hyunbin Lee[1], Grace Nye[1], Eugene V Koonin[2], Alex Gao[1], Wah Chiu[1], Rhiju Das[1]
[1]Stanford University, Stanford, CA, USA. [2]National Institutes of Health, Bethesda, MD, USA

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9:10 - 9:30am
**430 Discovery and characterization of substrate- and product-selective nylon hydrolases**
Nikolas Capra[1], Liangyu Qian[1], Célestin Bourgery[1], John F Cahill[1], Alexis Williams[1], Dana Carper[1], Jerry Parks[1], Isaiah T Dishner[1], Jeffrey C Foster[1], Delyana Vasileva[1], Serena Chen[1], Joshua Michener[1], Flora Meilleur[1,2]
[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]North Carolina State University, Raleigh, NC, USA

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9:30 - 10:00am

**262 X-ray Structure Analysis of a Novel 1C Metabolism Pathway in *Sphingobium lignivorans* SYK-6: Cooperative Function of LigM and S6MTHFR**

Professor Toshiya Senda PhD[1], Researcher HongYang Yu PhD[1], Associate Professor Naofumi Kamimura PhD[2], Professor Eiji Masai PhD[2]

[1]KEK, Tsukuba, Ibaraki, Japan. [2]Nagaoka University of Technology, Nagaoka, Niigata, Japan

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10:30 - 10:50am

**317 Structural basis for the conformational protection of nitrogenase from $O_2$**

Sarah M Narehood M.Sc.[1], Dr. Brian D Cook PhD[1], Dr. Suppachai Srisantitham PhD[1], Vanessa Eng M.Sc.[1], Dr. Angela A Shiau PhD[2], Dr. Kelly L McGuire PhD[1], Dr. R. David Britt PhD[2], Dr. Mark A Herzik PhD[1], Dr. F. Akif Tezcan PhD[1]

[1]University of California, San Diego, La Jolla, CA, USA. [2]University of California, Davis, Davis, CA, USA

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10:50 - 11:10am

**364 Atypical Structure Revealed In Carbohydrate Deacetylase Unique to Bacteroides**

Krystle J McLaughlin PhD[1], Lilith A Schwartz[1], Jordan O Norman[1], Sharika Hasan[1], Olive E Adamek[1], Elisa Dzuong[1], Jasmine C Lowenstein[1], Olivia G Yost[1], Banumathi Sankaran PhD[2]

[1]Vassar College, Poughkeepsie, NY, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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11:10 - 11:30am

**96 DNA binding and cleavage mechanism of DNA topoisomerase VI, an evolutionary counterpart of Spo11/Wadjet/Gabija systems**

Daniel E Richman[1], Timothy J Wendorff[1], Fahad Rashid[1], Curtis Beck[1], Matthew L Baker[2], Jonathan M Fogg[2], Lynn Zechiedrich[2], James M Berger[1]

[1]Dept of Biophysics and Biophysical Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD, USA. [2]Dept of Molecular Virology and Microbiology, Baylor College of Medicine, Houston, TX, USA

## 2.1.3 Innovations in Algorithms and Computational Methods

8:30 - 11:30am Sunday, 20th July, 2025

Session Room: Lilac AC

Chairs Alexis Rohou, Joseph 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.

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8:35 - 8:55am

**124 Leveraging generative modeling to analyze multiple related cryo-EM datasets**

Maria V Carreira[1], Laurel F Kinman[2], Joseph H Davis[1]

[1]MIT, Cambridge, MA, USA. [2]UCSF, San Francisco, CA, USA

8:55 - 9:15am

**50 Structure Determination in Cell Slices using 2D Template Matching**

Johannes Elferich[1], Stephen Diggs[1], Lingli Kong[1], Emily Plumb[2], Robert Arkowitz[2], Nikolaus Grigorieff[1]

[1]UMass Chan Medical School, Worcester, MA, USA. [2]Université Côte d'Azur, Nice, Alpes-Maritimes, France

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9:15 - 9:35am

**230 Two-Dimensional Template Matching (2DTM) enables accurate identification and probing of macromolecular structure within *in situ* cryo-EM datasets.**

Mr Matthew Giammar, Dr Joshua Dickerson, Prof Bronwyn Lucas

UC Berkeley, Berkeley, CA, USA

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9:35 - 10:00am

**397 Advancing Particle Identification in Cryo-Electron Tomograms with Deep Learning**

Jonathan Schwartz, Saugat Kandel, Hannah Siems, Clinton S Potter, Daniel Serwas, Bridget Carragher, Shawn Zheng, Dari Kimanius

Chan Zuckerberg Imaging Institute, Redwood City, CA, USA

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10:30 - 10:50am

**208 Analytical Differentiable Finite-Resolution Density Map Calculation in CCTBX/Phenix**

Dr Pavel Afonine PhD[1], Dr Paul Adams PhD[1], Prof Alexandre Urzhumtsev PhD[2]

[1]LBNL, Berkely, CA, USA. [2]IGBMC, Strasbourg, Illkirch, France

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10:50 - 11:10am

**140 DMcloud: A Local Fitting Method for Accurate Structure Modeling in Medium to Low Resolution Cryo-EM Maps**

Genki Terashi Ph.D[1], Xiao Wang Ph.D[2], Yuanyuan Zhang[1], Han Zhu[1], Daisuk Kihara Ph.D[1]

[1]Purdue University, West Lafayette, Indiana, USA. [2]University of Washington, Seattle, Washington, USA

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11:10 - 11:30am

**104 AlphaFold as a Prior: Guiding Protein Structure Prediction Using Experimental Data with ROCKET**

Alisia Fadini[1], Minhuan Li[2], Airlie J. McCoy[1], Thomas C. Terwilliger[3], Randy J. Read[1], Doeke Hekstra[2], Mohammed AlQuraishi[4]

[1]University of Cambridge, Cambridge, Cambridgeshire, United Kingdom. [2]Harvard University, Cambridge, Massachusetts, USA. [3]New Mexico Consortium, Santa Fe, New Mexico, USA. [4]Columbia University, New York City, New York, USA

### 2.1.4 Crystal Engineering

8:30 - 11:30am Sunday, 20th July, 2025

Session Room: Magnolia BC

Chairs Veronica Carta, Dan Decato

The intentional design and assembly of crystalline materials to control their physical and chemical properties (aka Crystal Engineering) is an interdisciplinary field. This session will

encompass various experimental and theoretical topics centered on solid-state assembly including, but not limited to, supramolecular interactions, multicomponent crystal systems, polymorphism, and the mechanical properties of crystalline materials. The session aims to balance translational and fundamental studies showcasing the versatility and impact of crystal engineering across disciplines.

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8:30 - 9:00am
**257 Structurally Diverse Small Molecule Quasiracemates**
Kraig Wheeler, Kamrynn Burk, Noah Dunham, Ainsley Hill, Molly Fleagle, Shay Perlot, Diana Schepens, Henry Zaske
Whitworth University, Spokane, WA, USA

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9:00 - 9:30am
**265 Crystal engineering via mechanochemistry: Cocrystals, salts, and polymorphs**
Dr Delbert S Botes PhD, Dr Kristin Hutchins PhD
University of Missouri, Columbia, Missouri, USA

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9:30 - 10:00am
**377 What crystal engineering can teach us about water treatment.**
Senior Principal Scientist Michael A. Reynolds Ph.D.
Shell Catalysts and Technologies, Houston, Texas, USA

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10:30 - 10:50am
**255 Are these crystals isostructural? Symmetry requirements, extent of difference, and likeness of supramolecular interactions**
Dr Petra Bombicz PhD
Centre for Structural Science, HUN-REN Research Centre for Natural Sciences, Budapest, Budapest, Hungary

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10:50 - 11:10am
**120 Engineering Multifunctional Surfaces: Unveiling the Extraordinary Electrical, Thermal, and Magnetic Properties of CVD-Synthesized Carbon Nanotubes via Nanofabrication**
Dr Salah OUDJERTLI Habilitation to Direct Research and Senior Researcher Class- A -
Research Center in Industrial Technologies. (CRTI) BP 64, Roade of Dely Brahim, Cheraga, 16014 Algiers – Algeria, Algiers, Algeria, Algeria

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11:10 - 11:30am
**15 Crystal Engineering of Nucleic Acid Macro-molecules using Selenium Atoms**
Prof. Zhen Huang Ph.D.[1], Hehua Liu Ph.D.[1], Jianhua Gan Ph.D.[2]
[1]SeNA Research Institute, College of Life Sciences, Hubei University, Wuhan, Hubei, China.
[2]School of Life Sciences, Fudan University, Shanghai, Shanghai, China

**2.1.5 Applications, Advances and Challenges with Total Scattering for Disorder Studies**
8:30 - 11:30am Sunday, 20th July, 2025
Session Room: Lilac B
Chairs Danielle Alverson, Yuanpeng Zhang

Total scattering encompasses both Bragg and diffuse scattering, enabling data analysis and modeling to extract structural information from both an average and local perspective. Since the resurgence of total scattering in the late 1980s, there has been a continuous emphasis on studying local disorder in various functional materials. This session aims to showcase recent applications of total scattering in investigating local disorder in energy storage materials, catalysts, magnetic systems, and other areas of interest. Furthermore, the session will explore recent and future advancements and challenges in instrumentation, data processing, analysis methodologies, and software tools. As the total scattering community continues to expand, this platform seeks to foster education, communication, and envision the future of the field.

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8:30 - 8:55am

**12 Local Symmetry Broken, Global Spins Aligned: Co-Emergence of Local Distortions and Antiferromagnetism in the Kagome Magnet ($Fe_{0.55}Co_{0.45}$)Sn**

Tsung-Han Yang

Oar Ridge National Laboratory, Oak Ridge, TN, USA

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8:55 - 9:15am

**150 Neutron Total Scattering Experiments at High Pressure: Measuring Crystalline Structural Heterogeneity using the SNAP Instrument at the Spallation Neutron Source**

John Hirtz[1], Cale Overstreet[1], Eric C O'Quinn[1], Maik K Lang[1], A. M. dos Santos[2], Matthew Tucker[2]

[1]University of Tennessee, Knoxville, TN, USA. [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA

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9:15 - 9:35am

**387 Harnessing Total Scattering Techniques to Examine Local and Average Structure in Li/Mn Rich Cathodes**

Megan Murphy[1], Jue Liu[1], Boyu Shi[2], Gihan Kwon[3], Subhadip Mallick[2], Eungje Lee[2], Jason Croy[2], Michael Thackeray[2], Mahalingam Balasubramanian[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]Argonne National Laboratory, Lemont, IL, USA. [3]Brookhaven National Laboratory, Upton, NY, USA

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9:35 - 10:00am

**85 Hydride ions in Group II Metal (A = Ca, Sr, Ba) Titanate Oxyhydrides**

Kennedy Agyekum[1], Dr. Bernadette Cladek[1], Megan Burrill[2], Dr. Jue Liu[3], Dr. Katharine Page[1,3]

[1]University of Tennessee, Knoxville, Knoxville, Tennessee, USA. [2]Northwestern University, Evanston, Illinois, USA. [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

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10:30 - 10:50am

**7 The Mechanism of Fluorine Doping for the Enhanced Lithium Storage Behavior in Cation-Disordered Cathode Oxide**

Dr. Yuanpeng Zhang PhD

ORNL, Oak Ridge, TN, USA

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10:50 - 11:10am

**160 High-Quality PDF Data Collection with a Ag source Single Crystal X-ray Diffractometer**

Ashley (Weiland) Schmidt PhD
Bruker AXS, Madison, WI, USA

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11:10 - 11:30am
**333 Noble Precision: Advancements in Silver (Ag) Radiation for X-ray Crystallography**
Michael Ruf Dr.[1], Ashley Schmidt PhD[1], Tobias Stürzer Dr.[2]
[1]Bruker AXS, LLC, Madison, WI, USA. [2]Bruker AXS SE, Karlsuhe, BW, Germany

**2.1.6 Combining experimental data with predicted models for structure determination**
8:30 - 11:30am Sunday, 20th July, 2025
Session Room: Lilac D
Chairs Rakhi Rajan, Christopher Williams
This session focuses on the integration of crystallographic data with predicted models obtained from AI-driven tools like AlphaFold and RosettaFold. Abstracts should highlight methodologies and best practices for combining experimental data and predicted models to improve the structure determination workflow. The session also welcomes case studies demonstrating the application and benefits of these combined techniques in resolving biological structures.

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8:30 - 9:00am
**239 Computing the human interactome**
Dr. Jing Zhang[1], Dr. Ian Humphreys[2], Dr. Jimin Pei[1], Dr. Qian Cong[1]
[1]University of Texas Southwestern Medical Center, Dallas, TX, USA. [2]University of Washington, Seattle, WA, USA

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9:00 - 9:30am
**331 Modeling is Believing? How AlphaFold2 Can Mislead Molecular Interpretation**
Karly Forker[1], Matthew C Fleming PhD[2], Kenneth H Pearce PhD[2], Cyrus Vaziri PhD[2], Albert Bowers PhD[2], Pei Zhou PhD[1]
[1]Duke University, Durham, NC, USA. [2]University of North Carolina Chapel Hill, Chapel Hill, NC, USA

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9:30 - 10:00am
**350 Improving Signal-to-Noise Ratio of Drug Fragment Screening with Variational Autoencoder**
Phyllis Zhang[1], Dr. Minhuan Li Ph.D.[2,3], Dr. Daniel Keedy Ph.D.[4], Dr. Tamar Skaist Mehlman Ph.D.[4], Dr. Doeke Hekstra Ph.D.[2]
[1]Harvard College, Cambridge, MA, USA. [2]Harvard University, Cambridge, MA, USA. [3]Flatiron Institute, New York City, NY, USA. [4]CUNY Advanced Science Research Center, New York City, NY, USA

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10:30 - 11:00am
**308 Predictive modeling and x-ray crystallography for mechanistic understanding of GO DNA repair**
Dr. Martin P Horvath PhD[1], Melody Malek[2], Danielle Yama[1], Dr. Carlos Trasviña-Arenas PhD[2,3], Dr. Sheila S David PhD[2]
[1]University of Utah, Salt Lake City, Utah, USA. [2]University of California Davis, Davis, California, USA. [3]Cenvistav, Mexico City, Ciudad de México, Mexico

11:00 - 11:30am

**248 When does structure modeling go wrong? A PDB-scale analysis of protein structure model validation using DAQ Score**

Daisuke Kihara PhD[1,2], Tsukasa Nakamura Ph.D.[2,1], Genki Terashi Ph.D.[1]

[1]Purdue University, West Lafayette, IN, USA. [2]KEK, Tsukuba, Ibaragi, Japan

**PL2 Robert Bau Award: Dr. Craig Brown**

11:45am - 12:45pm Sunday, 20th July, 2025

Session Room: Junior Ballroom C

Dr. Craig M. Brown, NIST Fellow and Director of the Center for High-Resolution Neutron Scattering (CHRNS), has been named the recipient of the Kenneth N. Trueblood Award. This award recognizes exceptional contributions to chemical crystallography and honors the legacy of Professor Kenneth N. Trueblood's impact on structural science.

Dr. Brown leads the Structure and Dynamics of Materials team at the NIST Center for Neutron Research and serves as an Adjunct Professor of Chemical Engineering at the University of Delaware. His work focuses on the structural and dynamical characterization of energy-related materials, including applications in hydrogen storage and small molecule separations. He has published over 250 scientific papers and is widely recognized in the field.

Dr. Brown's collaborative research spans DOE national labs and academic institutions. His accolades include the NIST Samuel Wesley Stratton Award, the DOE Hydrogen and Fuel Cells Program R&D Award, the Neutron Scattering Society of America Science Prize, the Arthur S. Flemming Award, the Department of Commerce Silver Medal, and the Presidential Early Career Award for Scientists and Engineers (PECASE).

**310 Adsorption and separations of small molecules in porous media**

Dr. Craig M Brown

NIST Center for Neutron Research, Gaithersburg, MD, USA

**DEI-2A #IAmRemarkable - PREREGISTRATION REQUIRED**

12:45 - 1:45pm Sunday, 20th July, 2025

Session Room: Cypress A

Chairs Alexis Davidson, Alice Thwin, Sandra Gabelli

#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

**DEI-2B #IAmRemarkable - PREREGISTRATION REQUIRED**

12:45 - 1:45pm Sunday, 20th July, 2025

Session Room: Cypress B

#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

**Industry Sponsored Lunch & Learn (Ticket Required)**
12:45 - 1:45pm Sunday, 20th July, 2025
Session Room: Lilac B
Join us for a special sponsored workshop hosted in partnership with Excillum, Proto, and DECTRIS. This engaging session will offer valuable insights and hands-on expertise from leaders in the field. *Please note: attendance is by invitation only.* Tickets are required and can be picked up directly from the booths of Excillum, Proto, or DECTRIS in the exhibit hall. Be sure to stop by early—space is limited and tickets will be distributed on a first-come, first-served basis.

**2.2.1 Emerging Modalities in Pharma Part 2**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Junior Ballroom C
Chairs Elizabeth Sprague, Susmith Mukund
This session will focus on the application of cryo-EM, x-ray crystallography and complementary biophysical and computational methods to the discovery and optimization of various drug modalities. For decades, small molecules by far have been the preferred modality to tackle diseases. While the past couple of decades have seen an exciting influx of transformative therapeutic antibodies, today, several other "non-standard" entities such as PROTACs, antibody-like scaffolds, macrocycles, peptides, covalent modulators, to name a few, are being developed to address unmet medical needs. We welcome submissions showcasing relevant structural biology techniques to drug discovery.

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2:00 - 2:20pm
**158 WRN helicase structural flexibility showcased through fragment-based lead discovery of inhibitors**
Rachel L Palte PhD[1], Mihir Mandal[2], Justyna Sikorska[2], Artjohn Villafania[2], Meredith M Rickard[1], Robert Bauer[1], Xiaomei Chai[1], Jiafang He[2], Zahid Hussain[2], Markus Koglin[2], Hannah B MacDonald[3], My S Mansueto[1], Klaus Maskos[4], Joey L Methot[1], Aileen Soriano[2], Marcel J Tauchert[4], Sriram Tyagarajan[2], Minjia Zhang[1], Daniel J Klein[5], Jacqueline D Hicks[2], David G McLaren[2], Sandra B Gabelli[5], Daniel F Wyss[2]
[1]Merck & Co., Inc., Boston, MA, USA. [2]Merck & Co., Inc., Rahway, NJ, USA. [3]MSD, London, England, United Kingdom. [4]Proteros Biostructures, Planegg-Martinsied, Germany, Germany. [5]Merck & Co., Inc., West Point, PA, USA

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2:21 - 2:40pm
**141 Structural basis of lipid-droplet localization of 17-beta-hydroxysteroid dehydrogenase 13**
Associate Research Fellow Shenping Liu Dr
Pfizer, Groton, CT, USA

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2:41 - 3:00pm
**206 Structural insights into mechanisms underlying stabilization of a lysosomal enzyme through protein engineering**

Jennifer E Kung, Ahlam Qerqez, Tianao Yuan, Lionel Rouge, Ann Nguyen, Oliver Davis, Cathal Mahon
Denali Therapeutics, South San Francisco, CA, USA

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3:30 - 3:45pm
**292 Validating Ligands with Phenix**
Dr Dorothee Liebschner PhD
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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3:46 - 4:00pm
**74 Improving macromolecular models of challenging ligands through combined QM/MM X-ray refinement**
Margarita A Tararina PhD[1], Lance M Westerhoff PhD[2], Oleg Borbulevych[2], Matt Pokross[1], David A Critton[1]
[1]Bristol Myers Squibb, Princeton, NJ, USA. [2]QuantumBio, Inc., State Collete, PA, USA

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4:01 - 4:20pm
**303 AMG193: Discovery and Structural basis for MTA cooperative inhibition of PRMT5*(Work done at Amgen with PRMT5 Team)***
Susmith Mukund
Independent Consultant, Foster City, CA, USA

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4:21 - 4:40pm
**36 X-ray crystallography reveals the mechanism of SARS-CoV-2 PLpro dimerization mediated by a DNA-encoded library screening hit**
Orville Pemberton, Amanda M Nevins, Thomas E Frederick, Emily Nicholl, Myron Srikumaran, Jun Chen, Alla Korepanova, Vincent Stoll, Andrew Petros, Sujatha Gopalakrishnan, Justin Dietrich, Liliam Rios Cordero, David J Hardee, Teresa I Ng, Chaohong Sun
AbbVie, North Chicago, IL, USA

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4:41 - 5:00pm
**349 Cryo-EM structures of Nipah virus polymerases and high-throughput biochemical RdRp assay development enable anti-NiV drug discovery**
Ahmed Rohaim[1], Colin Deniston[2], Zhenhang Chen[3], Cosmo Buffolo[2], Tiffany Tsang[1], Lilli Xie[1], Michael DiDonato[2], Glen Spraggon[2], Matt Clifton[1], Nadine Jarrousse[1], Judith Straimer[1], Bo Liang[3]
[1]Novartis, Emeryville, California, USA. [2]Novartis, San Diego, California, USA. [3]Emory University, Atlanta, Georgia, USA

**2.2.2 A Hitchhiker's Guide to Peer Review**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Magnolia BC
Chairs Chun Hsing 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.

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2:00 - 2:30pm
**153 But CheckCif Said So!**
Mohammad T Chaudhry PhD, Justin A Newman PhD
Merck & Co., Inc., Rahway, NJ, USA

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2:30 - 3:00pm
**407 Insights from an early career faculty on peer review**
Dr. Chrystal Starbird
University of North Carolina at Chapel Hill, Chapel Hill, NC, USA

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3:30 - 4:00pm
**408 Don't Panic & Other Thoughts on Crystallographic Refereeing**
Christine M Beavers
Rigaku Corporation, Akashima, Tokyo, Japan. Rigaku Americas, The Woodlands, Texas, USA

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4:00 - 4:30pm
**399 Peer Reviewing for Early Career Faculty**
Dr. Kenneth C. Childers PhD
California State University, Fullerton, Fullerton, CA, USA

**2.2.3 Extreme Biology: Probing the Conformational Landscape and Data Collection outside of Standard Practice**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Magnolia A
Chairs Vivian Stojanoff, Silvia Russi
Modern technologies have brought new capabilities that allow us to explore a range of crucial questions starting with how extreme environments drive molecular adaptation and influence biological function in adverse settings. By exposing biological samples to a range of stresses like extreme heat, pressure, or acidity, we can discover previously unknown molecular states and their functional consequences. The vast array of genomic information offers a readily available and invaluable resource for a systematic study of the molecular effects of extreme conditions

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2:00 - 2:30pm
**213 Making waves in structure-based ligand discovery**
Dr. Justin T Seffernick PhD, Dr. Marcus Fischer PhD
St. Jude, Memphis, TN, USA

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2:30 - 3:00pm
**274 Squeezing Out Secrets: How Pressure Reveals Structural Dynamics Across Whole Proteomes**
Richard E Gillilan[1], Haley Moran[2], Evelyn Patterson[2,3], Shreya Palakurthi[4,2], Edgar Manriquez-Sandoval[5], Stephen Fried[2,5]

[1]Center for High Energy X-ray Sciences, Cornell University, Ithaca, NY, USA. [2]Department of Chemistry, Johns Hopkins University, Baltimore, Md, USA. [3]Department of Biology, Johns Hopkins University, Baltimore, Md, USA. [4]Department of Biomedical Engineering, Johns Hopkins University, Baltimore, Md, USA. [5]Department of Biophysics, Johns Hopkins University, Baltimore, Md, USA

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3:30 - 3:55pm
**216 Multi-Temperature Crystallography of Polyamine Biosynthesis Enzymes Reveals Differing Active Site Conformations at RT than 100K**
Jonathan A Clinger
Baylor University, Waco, TX, USA

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3:55 - 4:15pm
**360 Examining *E.coli* aspartate transcarbamoylase with high-pressure crystallography**
Neti Bhatt M.S.[1], Jaidyn Duhon[1], Michael Patterson Ph.D.[1], Stephen Meisburger Ph.D.[2], Nozomi Ando Ph.D.[1]
[1]Cornell University, Ithaca, NY, USA. [2]Cornell High Energy Synchrotron Source, Ithaca, NY, USA

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4:15 - 4:35pm
**420 Acoustic combinatorial crystallization generates huge 9216 crystallization library from 64 building blocks**
Alexei Soares PhD
Brookhaven National Laboratory, Upton, NY, USA

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4:35 - 5:00pm
**419 Crystallography Across Temperature Extremes: Insights into the Conformational Landscapes of Human Kinases**
Michael C Thompson
University of California, Merced, Merced, CA, USA

**2.2.4 General Interest II**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Lilac B
Chairs Matthew McLeod, Alexis Davidson, Andrew Howard
General Interest sessions provide a platform for topics of broad relevance to structural science or for presentations that do not align with the specific themes of other sessions. All presentations are chosen from submitted abstracts.

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2:00 - 2:20pm
**309 New and Updated Features in Phenix for Macromolecular Structure Determination**
Billy K Poon Ph.D.
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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2:20 - 2:40pm
**130 Advancing towards a "one-button" screening solution for Cryo-EM data acquisition with Smart EPU**
Edward Pryor[1], Holger Kohr[2], Julio Ortiz[2], Fanis Grollios[2]

[1]Thermo Fisher Scientific, Hillsboro, OR, USA. [2]Thermo Fisher Scientific, Eindhoven, NL, Netherlands

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2:40 - 3:00pm
**286 Recent Advances in Cryo Electron Microscopy and Tomography**
Dr Eliza Nieweglowska PhD[1], Dr Marc M.H. Storms PhD[2], Dr Matt Joens PhD[1]
[1]Thermo Fisher Scientific, Los Angeles, California, USA. [2]Thermo Fisher Scientific, Eindhoven, Noord Brabant, Netherlands

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3:30 - 3:50pm
**43 Development of a Cloud-Based Learning Module for Protein Crystallography**
Dr. Christopher Jurgenson Ph.D.
Delta State University, Cleveland, MS, USA

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3:50 - 4:10pm
**247 A crystal-clear path to promoting crystallography to undergraduate students**
Carlos A Marrufo, Susanna Huang Undergraduate
Georgia Institute of Technology, Atlanta, GA, USA

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4:10 - 4:35pm
**161 Using dose aware and unattended data collection modes on the variable and microfocus macromolecular crystallography beamline I04 at Diamond Light Source**
Dr Ralf Flaig, Dr Pierpaolo Romano, Dr David Aragao
Diamond Light Source, Didcot, Oxfordshire, United Kingdom

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4:35 - 5:00pm
**112 Data Analysis tools for the Compact X-ray Light Source and Compact X-ray Free Electron Laser facilities at Arizona State University**
Dr. Sabine Botha[1], Annelise Velarde[1], Gihan Ketawala[1], Eric Everett[1], Roberto Alvarez[1], Dr. Thomas D Grant[2], Dr. Richard A Kirian[1]
[1]Arizona State University, Tempe, AZ, USA. [2]University of Buffalo, Buffalo, NY, USA

**2.2.5 Quantum Materials: Synthesis and Characterization**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Lilac D
Chairs Duminda Liurukara, 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.

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2:00 - 2:24pm
**187 Problems and progress in the growth and understanding of kagome materials**
Michael A McGuire
Oak Ridge National Laboratory, Oak Ridge, TN, USA

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2:24 - 2:48pm

**260 Pentagonal all-in-all-out antiferromagnetic chains in $NaMn_6Bi_5$**

Madalynn Marshall[1], Raimundas Sereika[2], Wenli Bi[2], Randy S. Fishman[3], David S. Parker[3], Huibo Cao[4]

[1]Kennesaw State University, Kennesaw, Georgia, USA. [2]Department of Physics, University of Alabama, Birmingham, Alabama, USA. [3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [4]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

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2:48 - 3:00pm

**42 Neutron Scattering Study of a Frustrated Kagome-Strip Structure: $Na_2Co_3(AsO_4)_2(OH)_2$**

Emily D Williams[1], Dr. Duminda Sanjeewa[2], Dr. Stuart Calder[2], Dr. Tianran Chen[3]

[1]Clemson University, Clemson, South Carolina, USA. [2]Oak Ridge National Labratory, Oak Ridge, Tennessee, USA. [3]University of Tennessee, Knoxville, Tennessee, USA

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3:30 - 3:54pm

**117 Synthesis, Structure, and Magnetic Properties of Pseudo-One-Dimensional $\mu_3$-oxo Manganese (III) Phosphate Exhibiting Magnetization Steps at Low Temperatures**

Dr. Kulugammana Gedera Sanjaya Ranmohotti Ph.D

Governors State University, University Park, IL, USA

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3:54 - 4:18pm

**149 Investigating Quantum Materials with Half-Polarized Diffraction and magnetic PDF analysis at the HB-2A Neutron Powder Diffractometer**

Stuart Calder[1], Raju Baral[1], Matthew Powell[2], Joseph Kolis[2], Haidong Zhou[3]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]Clemson University, Clemson, SC, USA. [3]University of Tennessee, Knoxville, TN, USA

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4:18 - 4:32pm

**293 Short range magnetic correlations in van der Waals 2D materials analyzed using neutron scattering**

Raju Baral[1], Amanda A. Haglund[2], Jue Liu[1], Alexander I. Kolesnikov[1], David Mandrus[2], Stuart Calder[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]University of Tennesse, Knoxville, TN, USA

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4:32 - 4:46pm

**70 Atomic PDF analysis as a basis for calculating the electronic structure of quantum materials**

Professor Valeri Petkov Ph. D.

Central Michigan University, Mt. Pleasant, MI, USA

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4:46 - 5:00pm

**334 Tuning the magnetic properties of altermagnetic MnTe with pressure**

Edison P Carlisle, Benjamin A Frandsen PhD

Brigham Young University, Provo, UT, USA

**2.2.6 From Cells to Atoms – using CryoEM Approaches to address Biological Questions**
2:00 - 5:00pm Sunday, 20th July, 2025
Session Room: Lilac AC
Chairs Benjamin Barad, Juan Du
The ability to determine 3D structures of biological systems has skyrocketed due to recent advances in cryoEM. This section will focus on the use of single-particle cryo-EM and cryo-electron tomography to understand the molecular basis of biological processes.

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2:00 - 2:20pm
**234 Molecular Mechanisms of P2X Receptor Desensitization**
Dr. Steven E. Mansoor M.D., Ph.D.
Oregon Health & Science University, Portland, OR, USA

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2:20 - 2:40pm
**297 Towards quantitative analysis of conformational landscapes: benchmarking heterogeneous reconstruction tools in cryo-EM**
Laurel F. Kinman[1], Andrew V. Grassetti[2], Maria V. Carreira[2], Joseph H. Davis[2]
[1]UCSF, Department of Biochemistry & Biophysics, San Francisco, CA, USA. [2]MIT, Department of Biology, Cambridge, MA, USA

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2:40 - 3:00pm
**346 Structural Basis of Activity of and Resistance to HIV Integrase Inhibitors**
Associate Professor Dmitry Lyumkis
Salk Institute for Biological Studies, La Jolla, CA, USA

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3:30 - 3:52pm
**321 Structural mapping of mitochondrial co-translational import in cells**
Ya-Ting Chang[1], Dr. Benjamin A Barad Ph.D.[2], Juliette Hamid[3], Hamidreza Rahmani Ph.D.[1], Dr. Brian M Zid Ph.D.[3], Dr. Danielle A Grotjahn Ph.D.[1]
[1]Scripps Research Institute, La Jolla, California, USA. [2]Oregon Health and Science University, Portland, Oregon, USA. [3]University of California-San Diego, San Diego, California, USA

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3:52 - 4:15pm
**267 Visualizing host-virus interactions at high resolutions *in situ***
Yong Xiong
Yale University, New Haven, CT, USA

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4:15 - 4:37pm
**296 Computational tools to facilitate in situ structure determination using cryo-ET**
Alberto Bartesaghi PhD
Duke University, Durham, NC, USA

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4:37 - 5:00pm
**277 A multiscale imaging approach to studying the harpoon-like invasion organelle from microsporidian pathogens**

Gira Bhabha[1], Nicolas Coudray[1], Mahrukh Usmani[1], Margot Riggi[2], Janet Iwasa[3], Damian C Ekiert[1], Rishwanth Raghu[4], Ellen Zhong[5], Harshita Ramchandani[6], Daija Bobe[7], Mykhailo Kopylov[7]
[1]Johns Hopkins University, Baltimore, MD, USA. [2]Max Planck Institute of Biochemistry, Munich-Martinsried, Bavaria, Germany. [3]University of Utah, Salt Lake City, UT, USA. [4]Princeton University, Princeton, New Jersey, USA. [5]Princeton University, Princeton, NJ, USA. [6]University of Michigan, Ann Arbor, MI, USA. [7]New York Structural Biology Center, New York, NY, USA

**PS2: Poster Session #2**
5:30 - 7:30pm Sunday, 20th July, 2025
Session Room: Exhibit Hall
Chairs Cora Lind-Kovacs, Tim Stachowski, Leighanne Gallington
Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don’t miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

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**456 Optimal TELSAM-Target Protein Linker Character is Target Protein-Dependent**
Maria Jose P Romo[1], Alihikaua Keliiliki[1], Jacob C Aerett[1], Joseph F Gonzalez[1], Ethan Noakes[1], Elijah W Wilson[1], Conrad Smith[1], Blake Averett[1], Dalton Hansen[1], Riley Nickles[1], Miles Bradford[1], Sara Soleimani[1], Tobin Smith[1], Supeshala Nawarathnage[1], Prasadika Samarwickrama[1], Ariel Kelsch[1], Derick Bunn[1], Cameron Stewart[1], Seth Brown[1], Tzanko I Doukov[2]
[1]Brigham Young University, Provo, Utah, USA. [2]Stanford Synchrotron Radiation Lightsource, Menlo Park, California, USA

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**459 pH-Tuning the State-of-the-Art TELSAM Crystallization Chaperone**
Undergraduate Researcher Miles J Bradford B.S.
Brigham Young University, Provo, UT, USA

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**21 Substoichiometry in the Ba-Cu and Ba-Cu-O phase diagrams**
Avinash Kiran, Justin L Andrews
Purdue university, West Lafayette, Indiana, USA

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**242 Automated Removal of Ice Rings in Crystallography Images Using Denoising Autoencoder**
Kevin Fang[1], Dr. Yang Ha[2]
[1]Stratford Preparatory, Santa Clara, CA, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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**425 Low-Temperature Synthesis and Characterization of Hybrid Heavy Metal Zero-Dimensional Cluster Compounds Containing Pt/Ir and Bi.**
Gayomi Kanchana Samarakoon Mudiyanselage BSc, Logan Schilling Undergraduate, Professor Sviatoslav Baranets PhD

Louisiana State Univesity, Baton Rouge, Louisiana, USA

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**406 Elucidation of the 3D Structures of two Human RNA Triple Helices using Cryo-EM**

Madeline M. Mousseau[1], Conner J. Langeberg[2], Jeffrey S. Kieft[3], Jessica A. Brown[1]
[1]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, USA. [2]Innovative Genomics Institute, University of California, Berkeley, CA, USA. [3]New York Structural Biology Center, New York, NY, USA

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**439 Does crossing the pond affect crystal quality?**

Christopher S. Campomizzi[1,2], M. Elizabeth Snell[1,2], Halina Mikolajek[3,4], James Sandy[3], Juan Sanchez-Weatherby[3], Gabrielle R. Budziszewski[1,2], Silvia Russi[5], Aina E. Cohen[5], Michael A. Hough[4], Sarah E.J. Bowman[1,2]
[1]University at Buffalo - Hauptman Woodward Research Institute, Buffalo, NY, USA. [2]Department of Biochemistry, Jacobs School of Medicine and Biomedical Sciences, SUNY Buffalo, Buffalo, NY, USA. [3]Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, England, United Kingdom. [4]The Research Complex at Harwell, Harwell Science and Innovation Campus, Didcot, England, United Kingdom. [5]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Stanford University, Menlo Park, CA, USA

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**460 Structural Characterization of the SARS-CoV-2 Replication and Transcription Complex**

Dr. Jennifer L Warnock Ph.D.[1], Dr. Sharique Khan Ph.D.[1], Dr. Wellington Leite Ph.D.[1], Dr. Susan Tsutakawa Ph.D.[2], Dr. Gregory Hura Ph.D.[2], Dr. Hugh O'Neill Ph.D.[1]
[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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**241 The invariant theory of chiral order parameters**

Carter R. Baldwin[1], Isaac R. Burkholder[1], Jeremy B. Ruebush[2], Harold T. Stokes[1], Branton J. Campbell[1]
[1]Brigham Young University, Provo, Utah, USA. [2]Brigham Young University Idaho, Rexburg, Idaho, USA

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**435 New Methods in RNA Structural Biology: TELSAM Protein Chaperone Crystallography Applications to Folded RNA**

Jacob C Averett, Miles Bradford, Blake Averett, Dalton Hansen, Dr. James D Moody
Brigham Young University, Provo, Utah, USA

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**465 Investigating Polymer Flipping and Lattice Disruptions in TELSAM-Facilitated Protein Crystallization**

Ethan Noakes, MJ Pedroza Romo, Joseph Gonzalez, Alihi Keliiliki, Eli Anderson, Dr. James D Moody
Brigham Young University, Provo, Utah, USA

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**287 Recent Advances in Cryo Electron Microscopy and Tomography**

Product Marketing Manager Marc M.H. Storms PhD[1], Sr. Sales Development Representative Eliza Nieweglowska PhD[2], Sr. Sales Development Representative Matt Joens PhD[2]
[1]Thermo Fisher Scientific, Eindhoven, Noord Brabant, Netherlands. [2]Thermo Fisher Scientific, Los Angeles, California, USA

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**443 Crystal and Electronic Structure of $Ba_{12}Ga_{15}As_{22}$**
Spencer Watts, Larissa Najera, Dr. Sviatoslav Baranets
Louisiana State University, Baton Rouge, Louisiana, USA

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**155 EMSuite Server: Advanced Tools for Cryo-EM Structure Modeling, Validation, and Refinement**
Joon Hong Park[1], Javad Baghirov[2], Xiao Wang[3], Genki Terashi[1], Han Zhu[1], Yuki Kagaya[1], Pranav D Punuru[1], Shu Li[1], Devashish Prasad[1], Daisuke Kihara[1]
[1]Purdue University, West Lafayette, Indiana, USA. [2]University of Maryland, College Park, Maryland, USA. [3]University of Washington, Seattle, Washington, USA

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**271 Hexamer structure of *Pseudomonas aeruginosa* deoxynucleotide triphosphate triphosphohydrolase and its involvement in catalysis and DNA binding**
Han Byeol Oh, Sung-il Yoon
Kangwon National University, Chuncheon, Kangwon, Korea, Republic of

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**444 Antagonist development for the CMG2 protein**
Ms Prasadika Samarawickrama Hetti Arachchige PhD, Ms Fang Fang, Dr James David Moody, Dr Ken Christensen
Brigham Young University, Provo, Utah, USA

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**455 Optimizing TELSAM Fusion Constructs for Enhanced Protein Crystallization: Effects of Display Density and His Tag Configuration**
Ms Prasadika Samarawickrama Hetti Arachchige, Mr Kyle Ludlow, Mr Dallin Mead, Ms Alexis Xiong, Dr James Moody
Brigham Young University, Provo, Utah, USA

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**458 Crystallization of VPS34 with Small Molecule Drug Candidates**
Dr. James D Moody, Wisdom Abiodun, Evan Tsubaki
Brigham Young University, Provo, Utah, USA

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**110 Systematic metabolite screening identifies orthosteric and allosteric regulators of the adenosine A2A receptor**
Prashant Rao PhD[1], Manoj Rathinaswamy PhD[1], Michelle Chan[1], Kevin Hicks[2], Amirhossein Mafi PhD[1], Qi Hao PhD[1]
[1]Calico, San Francisco, California, USA. [2]University of Utah, Salt Lake City, UT, USA

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**306 Spatially resolved anomalous dispersion method for determination of site-specific oxidation states in metalloenzymes at XFEL sources**
Natalie M Minnetian PhD, Nicholas K Sauter PhD, Jan F Kern PhD
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

**251 Rising STARS: Developing Youth Engagement in Crystallography**

Mirah Lindsay[1], Susanna Huang[2]

[1]Walton High School, Atlanta, Georgia, USA. [2]Georgia Institute of Technology, Atlanta, GA, USA

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**389 Integration of experimental data with model prediction and simulation reveals how Mettl15-Mettl17 modulates pre-mitoribosome.**

Prof Alexey Amunts

Munster University, Munster, Germany, Germany

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**415 A structure-based high-efficiency homogeneous antibody platform by endoglycosidase Sz provides insights into its transglycosylation mechanism**

Prof. Chun-Jung Chen Ph.D.

National Synchrotron Radiation Research Center, Hsinchu, N/A, Taiwan

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**474 Re-thinking of the adhesion mechanism of Serine-aspartate repeat-containing protein D (SdrD)**

Dr. Younhchang Kim PhD[1], Ms. Angela Tan BS[2], Dr. Priyanka Gade PhD[1], Mr. Mike Enders MS[1], Dr. Xiaobing Zuo PhD[1], Dr. Kemin Tan PhD[1], Dr. Andrzej Joachimiak PhD[1]

[1]Argonne National Laboratory, Lemont, Illinois, USA. [2]University of Massachusetts Amherst, Amherst, Massachusetts, USA

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**481 From Resolution to Revolution: Cryo-EM Driven Advances in Structure-Based Drug Design for Membrane Proteins and Targeted Protein Degradation**

Victoria Ouroutzoglou

Viva Biotech, Cambridge, MA, USA

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**335 Grazing-Incidence X-ray Scattering at High Energies: Advanced Capabilities at the 11-ID Beamlines of the APS-U**

Justin M Hoffman, Olaf J Borkiewicz, Wenqian Xu, Andrey A Yakovenko

Argonne National Laboratory, Lemont, IL, USA

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**482 Crystallographic characterization and polymorphism in a calcium-based porphyrinic MOF with biomedical potential**

Dr Christelle N. Dzesse T., Dr Mario Wriedt

University of Texas at Dallas, Richardson, Tx, USA

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**494 Differentiating the Oxidation States of Copper in a Type-I Copper Protein Using XANES Spectra in the Crystalline State: A Comparison with Single-Crystal X-ray Crystallography Study**

Narayanasami Sukumar PhD[1], Sahana L Sukumar BS[2], George E Sterbinsky PhD[3]

[1]Cornell University, Argonne, Illinois, USA. [2]Loyola University, Chicago, Illinois, USA. [3]Argonne National Laboratory, Argonne, Illinois, USA

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**507 Using phase diagrams with microseeding to prepare crystal samples for advanced data collection techniques**

Mr Patrick D Shaw Stewart m.Phil.[1], Mr. Stefan A `Kolek B.Sc.[1], Mr. Jack R Stubbs B.Sc.[2], Mr. Peter F M Baldock B.Sc.[1]
[1]Douglas Instruments Ltd, Hungerford, Berkshire, United Kingdom. [2]University of Southampton, Southampton, Hampshire, United Kingdom

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**485 Engineering Site-Specific Fluorescently-Labeled IEPs to Monitor Group II Intron RNP Assembly**

Jasmine A Harper, Sarah A Starcovic, Dr Neil Billington, Dr Aaron R Robart
West Virginia University, Morgantown, WV, USA

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**510 Structural Insights into the Mechanism of Bacteriophage Mu Transposition**

Dr Juhi Singh phD[1], Prof Phoebe A Rice phD[2]
[1]University of Chicago, Chicago, Illinois, USA. [2]University of Chicago, Chicago, Illinoise, USA

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**513 Structural insights into the inhibition of *M. tuberculosis* Prolyl-tRNA synthetase by derivatives of 3-aminopyrazine-2-carboxamide**

Priyanka Gade[1,2], Karolina Michalska[1,2], Vinod Sukanth Kumar Pallabothula[3], Jan Zitko[3], Andrzej Joachimiak[1,2,4]
[1]Center for Structural Biology of Infectious Diseases, Consortium for Advanced Science and Engineering, University of Chicago, Chicago, Illinois, USA. [2]Structural Biology Center, X-ray Science Division, Argonne National Laboratory, Lemont, Illinois, USA. [3]Faculty of Pharmacy in Hradec Králové, Charles University, Ak. Heyrovského 1203/8, 500 05 Hradec Králové, Czech Republic. [4]Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, Illinois, USA

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**514 Recent advances and upgrades in the advanced crystallographic program at NSF's ChemMatCARS**

Dr. Jinxing Jiang PhD[1], Dr. Tieyan Chang PhD[2], Kevin Lynch[2], Dr. Yu-Sheng Chen PhD[2]
[1]University of Illinois at Chicago, Chicago, IL, USA. [2]The University of Chicago, Chicago, IL, USA

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**500 Observation of Ras protein GTP hydrolysis and conformation change by freeze-trap serial X-ray crystallography**

Dr. Takashi Kawamura Ph.D.[1], Dr. Wakako Sakisaka Ph.D.[2], Dr. Yoshiteru Makino Ph.D.[2], Dr. Shigeyuki Matsumoto Ph.D.[3], Dr. Yoko Yoshikawa Ph.D.[2], Dr. Kazuya Hasegawa Ph.D.[1], Dr. Fumi Shima Ph.D.[2], Dr. Takashi Kumasaka Ph.D.[1]
[1]Japan Synchrotron Radiation Research Institute, Sayo-cho, Sayo-gun, Hyogo, Japan. [2]Graduate School of Science, Technology and Innovation, Kobe University, Kobe, Hyogo, Japan. [3]Graduate School of Medicine, Kyoto University, Kyoto, Kyoto, Japan

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**73 Crystallization of ExoR - $His_6$, A Regulatory Signal Controlling Symbiotic Nitrogen Fixation**

Katherine Lee, Dr. Kenneth Childers Ph.D., Dr. Madeline Rasche Ph.D.
California State University Fullerton, Fullerton, CA, USA

**Fellows Reception INVITE ONLY**
6:00 - 8:00pm Sunday, 20th July, 2025
Session Room: Junior Ballroom B
The ACA Fellows Reception is a special evening dedicated to recognizing the outstanding contributions of our Fellows to the field of crystallography. This event offers an opportunity for Fellows and invited guests to connect in an informal setting, celebrate achievements, and foster community within the ACA.

Light refreshments and hors d'oeuvres will be served. We encourage all ACA Fellows to attend and join us in honoring this distinguished group.

**2.3.1 Would You Publish This**
7:30 - 9:30pm Sunday, 20th July, 2025
Session Room: Junior Ballroom C
Chairs Scott Lee, Gerald Audette, Storm Dragonson
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!

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7:35 - 7:45pm
**60 Is it new or wrong? Responsibility in reporting novel structures.**
Glenn P Yap Ph.D.
University of Delaware, Newark, DE, USA

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7:45 - 7:55pm
**109 : "I'm sorry, Dave, I'm afraid I can't do that" Part 2**
Professor David R. Rose
University of Waterloo, Waterloo, Ontario, Canada

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7:55 - 8:05pm
**144 Responding to CheckCIF "Experts"**
Carla Slebodnick[1], Abigail Edwards[2], Landon J. Elkins[2], Tegan A. Makal[2]
[1]Department of Chemistry, Virginia Tech, Blacksburg, VA, USA. [2]Department of Natural Sciences, The University of Virginia's College at Wise, Wise, VA, USA

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8:05 - 8:15pm
**281 Is it Ever Acceptable to SQUEEZE Charge Balance?**
Dr. Toby J Woods Ph.D.
University of Illinois at Urbana-Champaign, Urbana, IL, USA

8:15 - 8:25pm
**304 Two problematic structures: partial residual electron density in a crown ether and cages with 4 metal centers and 8 disordered anions.**
Veronica Carta
UC Riverside, Riverside, CA, USA

**Bragg About It: Karaoke Night**
8:00 - 10:00pm Sunday, 20th July, 2025
Session Room: Magnolia A
Looking to unwind and have some fun? Join for a Karaoke & Board Games Night!

Whether you're ready to belt out your favorite power ballad, dominate in Codenames, or just hang out with fellow structural science enthusiasts, we've got something for you.

Come solo or bring your friends—everyone is welcome!

**Registration Desk**
7:30am - 5:00pm Monday, 21st July, 2025
Session Room: Grand Ballroom Foyer

**Speaker Ready Room**
7:30am - 5:00pm Monday, 21st July, 2025
Session Room: Walnut

**3.1.1 Managing High Data Rates in Structural Science**
8:30 - 11:30am Monday, 21st July, 2025
Session Room: Lilac D
Chairs Justyna Wojdyla, Vivian Stojanoff, Christine Beavers
This session invites abstracts that address the challenges and solutions associated with handling large volumes of crystallographic data. We seek contributions that explore techniques for processing high data rates, data compression methods, and scalable storage solutions. We also welcome submissions on best practices for long-term data archiving, integration of automated systems, and the use of cloud-based platforms to manage high-throughput crystallographic experiments. Abstracts implementing FAIR principles of making crystallographic data Findable, Accessible, Interoperable, and Reusable (FAIR) to improve reproducibility in research are also welcomed. These contributions could explore strategies and tools for implementing FAIR principles in data archiving, including metadata standards, data sharing platforms, best practices for data documentation and case studies where FAIR data archiving has improved reproducibility.

8:30 - 8:50am
**58 Climbing Mountains: Building a Data Capture and Correction System for JUNGFRAU 9M**
Dr Graeme Winter Ph.D[1,2,3], Dr Nick E Devenish Ph.D.[3], Mr James O'Hea[3], Mr Gary Yendell[3]
[1]NE-CAT, Lemont, IL, USA. [2]Cornell University, Ithaca, NY, USA. [3]Diamond Light Source, Didcot, Oxfordshire, United Kingdom

8:50 - 9:10am

**278 SBCloud: A Cloud-Based Platform for Structure Determination and Data Storage**

Jason M Key Ph.D[1], Benjamin Eisenbraun[1], Peter A Meyer Ph.D[1], Piotr Sliz Ph.D[1,2]

[1]Harvard Medical School, Boston, MA, USA. [2]Boston Children's Hospital, Boston, MA, USA

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9:10 - 9:30am

**127 PDBx/mmCIF Ecosystem: Foundation for FAIR Access to Macromolecular Structure Data**

Dr Brinda Vallat Ph.D.

RCSB PDB, Rutgers University, Piscataway, NJ, USA

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9:30 - 9:50am

**193 Navigating the Data Deluge at the SLS 2.0 Macromolecular Crystallography (MX) Beamlines**

Dr. Jiaxin Duan[1], Dr. Guillaume Gotthard[1], Dr. Vincent Olieric[1], Dr. Max Burian[2], Dr. Ludmila Leroy[2], Dr. Camilla Larsen[2], Dr. Meitian Wang[1], Dr. Filip Leonarski[1]

[1]PSI, Villigen, Aargau, Switzerland. [2]DECTRIS, Baden, Aargau, Switzerland

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9:50 - 10:00am

**359 The Cosmos and Crystal Connection: What We Can Learn About Data Compression**

Kimberly M. Horvat B.A[1,2], Dr. Herbert J. Bernstein PhD[3], Dr. Alexei S. Soares PhD[2], Dr. Jean Jakoncic PhD[2]

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

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10:30 - 10:50am

**203 Enabling Next-Generation Structural Science with Cloud and Edge Computing**

Max Burian PhD, Ludmilla Leroy, Fabian Eisenstein, Pascal Hofer

DECTRIS Ltd., Baden, AG, Switzerland

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10:50 - 11:10am

**102 Improving Data Representation of Metalloproteins in the Protein Data Bank**

Alison Biester[1], Chenghua Shao[1], Zukang Feng[1], Ezra Peisach[1], Jasmine Y. Young[1], wwPDB Team[1,2,3,4,5], Stephen K. Burley[1,6,7,8,9]

[1]RCSB Protein Data Bank and Institute for Quantitative Biomedicine, 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, Suita, Osaka, Japan. [4]EMDB, EMBL-European Bioinformatics Institute, Hinxton, Cambridge, United Kingdom. [5]BMRB, UConn Health, University of Connecticut, Farmington, CT, USA. [6]RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, San Diego, CA, USA. [7]Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ, USA. [8]Rutgers Cancer Institute, Rutgers, The State University of New Jersey, New Brunswick, NJ, USA. [9]Rutgers Artificial Intelligence and Data Science (RAD) Collaboratory, Rutgers, The State University of New Jersey, Piscataway, NJ, USA

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11:10 - 11:30am

**201 Toward Extreme Lossy Compression Data to Enable Higher Data Rates MX**
Dr Jean Jakoncic PhD[1], Dr Herbert J Bernstein PhD[2]
[1]Brookhaven National Laboratory, National Synchrotron Light Source II, Upton, NY, USA. [2]Fresh Pond Institute, Cambridge, MA, USA

### 3.1.2 General Interest III

8:30 - 11:30am Monday, 21st July, 2025
Session Room: Magnolia BC
Chairs Alexis Davidson, 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

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8:30 - 8:55am
**142 Structural Mechanism of a Partial Glucocorticoid Receptor Agonist Functioning as a Mineralocorticoid Receptor Antagonist**
Dr. Xu Liu Ph.D
Emory University, Atlanta, Georgia, USA

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8:55 - 9:15am
**159 The structural basis for synergistic inhibition of geranylgeranyl diphosphate synthase with stereoisomeric triazole bisphosphonates**
Andrew Pham, Sarah Holstein, Gloria Borgstahl
UNMC, Omaha, NE, USA

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9:15 - 9:35am
**192 Understanding the off-loading mechanism of adenosylcobalamin by *Cupriviadus metallidurans* adenosyltransferase from *C. metallidurans* Isobutyryl-CoA Mutase Fused**
Jayoh Amurao Hernandez PhD
MIT, Cambridge, MA, USA

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9:35 - 10:00am
**199 The Ultrahigh-Resolution Protein Crystal Structure of Crambin**
Changsoo Chang[1], Julian C.H. Chen[2], Miroslaw Gilski[3,4], Dominika Borek[5], Zbyszek Otwinowski[5], Maciej Kubicki[4], Mariusz Jaskolski[4,3], Andrzej Joachimiak[1,6]
[1]Argonne National Laboratory, Lemont, IL, USA. [2]Los Alamos National Laboratory, Los Alamos, NM, USA. [3]Polish Academy of Sciences, Poznan, PL.WP, Poland. [4]Adam Mickiewicz University, Poznan, PL.WP, Poland. [5]The University of Texas Southwestern Medical Center, Dallas, TX, USA. [6]University of Chicago, Chicago, IL, USA

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10:30 - 10:50am
**243 Cryo-EM Structure of a Type I Anti-Prothrombin Antibody Reveals a Novel Kringle-1 Epitope and Its Functional Impact**
Suresh Kumar PhD, Nicola Pozzi PhD
Saint Louis University, Saint Louis, Missouri, USA

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10:50 - 11:10am

**429 Structural insights of anti-MHC-I monoclonal antibodies that block NK cell receptor interactions with tumors**

Dr. Jiansheng Jiang Ph.D.[1], Dr. Kannan Natarajan Ph.D.[1], Dr. Abir Panda[1], Lisa F. Boyd[1], Reanne Towler[1], Dr. Haotian Lei[1], Dr. Rick Huang[2], Dr. Ethan M. Shevach[1], MD. Ph.D. David H. Margulies[1]

[1]NIAID/NIH, Bethesda, Maryland, USA. [2]CCR/NCI, Bethesda, Maryland, USA

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11:10 - 11:30am

**139 Muscle acetylcholine receptor high resolution structures: insights into development and autoimmune disease**

Huanhuan Li[1], Minh Pham[2], Jinfeng Teng[1], Kevin O'Connor[2], Colleen Noviello[1], Ryan Hibbs[1]

[1]University of California San Diego, La Jolla, CA, USA. [2]Yale University, New Haven, CT, USA

**3.1.3 Mathematical, Theoretical, and Computational Crystallography**

8:30 - 11:30am Monday, 21st July, 2025

Session Room: Lilac B

Chairs Carolyn Brock, 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.

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8:30 - 8:55am

**405 New Computational Approaches to the Analysis of Single Crystal Diffuse Scattering**

Raymond Osborn PhD, Stephan Rosenkranz PhD, Matthew Krogstad PhD

Argonne National Laboratory, Lemont, IL, USA

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8:55 - 9:20am

**319 XsymNet: Combined Exhaustive Symmetry and Machine Learning for Phase Transition Studies**

Dr. Dayton G. Kizzire, Dr. Maksim Eremenko, Dr. Matt Tucker, Dr. Yuanpeng Zhang

Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

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9:20 - 9:40am

**240 Structure property relationships and symmetry-mode analysis of single-layered hybrid organic-inorganic perovskite compounds**

Isaac R. Burkholder[1], Cindy Y. Wong[2], Kameron R. Hansen[3], John S. Colton[1], Andre Schleife[2], Harold T. Stokes[1], Branton J. Campbell[1]

[1]Brigham Young University, Provo, Utah, USA. [2]University of Illinois Urbana-Champaign, Urbana, Illinois, USA. [3]University of Utah, Salt Lake City, Utah, USA

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9:40 - 10:00am

**305 Continuous symmetry measures: From point groups to space groups**

Dr Gil Alon Senior Lecturer

The Open University of Israel, Raanana, Israel, Israel

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10:30 - 10:50am

**320 Prevalence and Significance of Approximate Symmetry in *Z'* > 1 Orgainc Structures**

Professor Carolyn P Brock PhD
University of Kentucky, Lexington, KY, USA

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10:50 - 11:15am
**340 FINDEXER: a new technique to find unit cells in sparse serial patterns**
Daniel Paley, Aaron Brewster, David Mittan-Moreau, Nicholas Sauter
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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11:15 - 11:30am
**147 Theoritical Calculations in Structures and Functions of Proteins**
Dr. Yang Ha PhD
Lawrence Berkeley National Lab, Berkeley, CA, USA

**3.1.4 Quantum Crystallography: Latest Developments, Applications, and Experiences**
8:30 - 11:30am Monday, 21st July, 2025
Session Room: Magnolia A
Chairs Sylwia Pawledzio, Anna Krawczuk
This session is open to all scientists, from hands-on practitioners to experts in method development, and especially welcomes end-users of quantum crystallographic techniques to present their experiences and findings. Topics may encompass any theoretical or practical applications of quantum mechanics in the study of crystalline materials. Presenters are encouraged to demonstrate how these techniques enhance agreement with experimental data, leading to deeper material insights. Research areas can include inorganic solids, molecular networks, organic and organometallic compounds, as well as large structures like proteins.

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8:30 - 9:00am
**128 Advancing Protein Structure and Ligand Binding Studies with Quantum Crystallography**
dr Maura Malinska
University of Warsaw, Warsaw, mazowieckie, Poland

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9:00 - 9:30am
**87 Quantum Crystallographic tomography of electrons in phase space**
M. Sizhuo Yu[1], Prof Jean-Michel Gillet Dr[1], Jules Andrevon-Canut[2]
[1]CentraleSupelec, Gif sur Yvette, France, France. [2]Paris-Saclay University, Gif sur Yvette, France, France

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9:30 - 10:00am
**122 Quantum crystallography applied to RNA in Olex2**
Prof. Blaine H. M. Mooers PhD
University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

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10:30 - 11:00am
**19 Quantum Crystallography as a Chemist's Tool for Bond Analysis**
Floran Meurer M. Sc., Dr. Michael Bodensteiner Dr.
University of Regensburg, Regensburg, Bavaria, Germany

### 3.1.5 Flexibility, Dynamics & The Secret Lives of Proteins

8:30 - 11:30am Monday, 21st July, 2025

Session Room: Junior Ballroom C

Chairs Kara Zielinski, 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.

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8:31 - 9:00am

**231 Photoactivation in Myxobacterial Phytochrome: Early Events**

Emina A Stojkovic PhD[1], Tek N Malla PhD[2], Sebastian Westenhoff PhD[3], Marius Schmidt PhD[2]

[1]Northeastern Illinois University, Chicago, IL, USA. [2]University of Wisconsin-Milwaukee, Milwaukee, WI, USA. [3]Uppsala University, Uppsala, Sweden, Sweden

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9:00 - 9:30am

**332 Towards direct visualization of the reaction coordinates of proteins**

Dr Doeke R Hekstra PhD[1], Dr. BoRam Lee PhD[2], Dr. Rama Ranganathan PhD[2], Dr. Kristopher I White PhD[3], Dr. Margaret A. Klureza PhD[1], Dr. Jack B. Greisman PhD[1,4], Dr. Kevin M. Dalton PhD[5,6], Dr. Robert W Henning PhD[2], Dr. Vukica Srajer PhD[2]

[1]Harvard University, Cambridge, MA, USA. [2]University of Chicago, Chicago, IL, USA. [3]Stanford University, Stanford, CA, USA. [4]D.E. Shaw Research, New York, NY, USA. [5]SLAC National Lab, Menlo Park, CA, USA. [6]New York University, New York, NY, USA

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9:30 - 10:00am

**266 How Physiological Temperature Drives Ligand Recognition and Channel Gating**

Dr. Wei Lu PhD

Northwestern University, Evanston, IL, USA

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10:30 - 10:50am

**56 Atomic-Level Insights from SWAXS: Quantifying Uncertainty in Biological Models**

Patrick K. Oduro, Jitendra Singh, Dr. Sarah Chamberlain Ph.D., Dr. Thomas D. Grant Ph.D.

SUNY University at Buffalo, Buffalo, New York, USA

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10:50 - 11:10am

**307 Atomic Detail from Disordered Regions: QM/MM-Based Real-Space Reconstruction of Loops, Rotamers, and Protonation States in X-ray/Cryo-EM Density**

Dr. Lance M Westerhoff PHD, Dr. Oleg Borbulevych PHD

QuantumBio Inc, State College, PA, USA

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11:10 - 11:30am

**376 Progress on the UNTANGLE Challenge for revealing cooperative motions**

Prof James M Holton PhD
UCSF, San Francisco, CA, USA

**3.1.6 Developments in Data Collection and Automation in MicroED**
8:30 - 11:30am Monday, 21st July, 2025
Session Room: Lilac AC
Chairs Shao-Liang Zheng, Brandon Mercado
MicroED has been at the forefront of expanding the possibilities of structure models accessible through crystallography. Numerous efforts have been dedicated to enhancing the pipeline for delivering these results. This session will explore advancements in automation, covering a wide range of topics. We will delve into general improvements in data collection strategies, as well as groundbreaking developments in truly autonomous, high-throughput approaches to MicroED. Additionally, we will discuss simultaneous compositional analysis of complex samples, further broadening the capabilities of MicroED. Join us in this session to discover the latest automation advances in microcrystal electron diffraction.

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8:30 - 9:00am
**233 Managing electron-counted MicroED data**
Johan Hattne[1,2], Michael W Martynowycz[2], Max T B Clabbers[2], William Nicolas[2], Tamir Gonen[1,2]
[1]Howard Hughes Medical Institute, Los Angeles, CA, USA. [2]University of California, Los Angeles, CA, USA

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9:00 - 9:30am
**386 Advancements in Electron Diffraction: A broad overview of the current state of ELDICO *ED-1* electron diffractometer and some case studies.**
Danny Stam MSc[1], Dr. Gustavo Santiso-Quinones pHd[2], Dr. Christian Jandl pHd[1], Dr. Johannes Merkelbach pHd[1], Laura Samperisi pHd[1]
[1]ELDICO Scientific AG, Allschwil, Basel-Land, Switzerland. [2]ELDICO Scientific AG, Allschwil, basel-land, Switzerland

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9:30 - 10:00am
**546 Standards for MicroED**
Johan Unge[1], Brent L Nannenga[1], Allen G Oliver[2], Tamir Gonen[3]
[1]Umeå University, Umea, Umea, Sweden. [2]University of Notre Dame, Notre Dame, IN, USA. [3]University of California,, Los Angles, CA, USA

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10:30 - 11:00am
**365 Semi-automated 3DED/microED data collection and processing unveil multiple polymorphs in biogenic guanine crystals from fish**
Dr. Naruhiko Adachi Ph.D
University of Tsukuba, Tsukuba, Ibaraki, Japan

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11:00 - 11:30am
**105 High-throughput electron diffraction in the XtaLAB Synergy-ED**
Dr. Robert Bucker[1], Mathias Meyer[2], Michal Jasnowski[2], Mateusz Idzi[2], Jessica Burch[3]
[1]Rigaku Europe SE, Neu-Isenburg, Neu-Isenburg, Germany. [2]Rigaku Oxford Diffraction, Wrocław, Wrocław, Poland. [3]Rigaku Americas, The Woodlands, TX, USA

**PL3 Fankuchen Award: Professor Chris D. Malliakas**
11:45am - 12:45pm Monday, 21st July, 2025
Session Room: Junior Ballroom C
Chris D. Malliakas will receive the ACA Fankuchen Memorial Award in recognition of his significant contributions to crystallographic research and his dedication to teaching in the field. As the Director of Crystallography, Director of Physical Characterization, and Research Associate Professor at the Integrated Molecular Structure Education and Research Center (IMSERC) at Northwestern University, Malliakas has demonstrated expertise in solving complex structural problems, including modulated structures, amorphous compounds, supercells, twinning, and disorders. His work extends beyond single-crystal analysis, having transformed structural elucidation capabilities at Northwestern University into a dynamic learning environment where he actively trains future structural scientists. His dedication to both advancing crystallographic methodologies and educating the next generation of researchers exemplifies the essence of the Fankuchen Award, which honors those who contribute to crystallographic research while being effective educators.

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**347 Learning, working, and teaching non-standard Crystallographic Techniques**
Prof Chris D. Malliakas PhD
Northwestern University, Evanston, IL, USA

**Private Event-Murphy**
11:45am - 1:45pm Monday, 21st July, 2025
Session Room: Cypress A

**APS Site Visit - PREREGISTRATION REQUIRED**
12:00 - 5:00pm Monday, 21st July, 2025
Session Room: Junior Ballroom B
**Important Note:**
Only participants who meet **all** of the following criteria will be permitted to enter Argonne National Laboratory:

*Are registered with the ACA
*Have completed all required APS security steps
*Arrive and depart using the ACA-provided transportation
*Present a REAL ID-compliant driver's license or a valid passport at the security checkpoint

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**Schedule & Transportation**

**PLEASE MEET PROMPTLY AT 12:00 PM IN JUNIOR BALLROOM B**

**12:30 PM – 12:45 PM** – Load buses at The Westin Chicago Lombard
*(70 Yorktown Shopping Center, Lombard, IL 60148)*
*A boxed lunch will be provided before departure.*
**12:45 PM – 1:15 PM** – Travel to Argonne National Laboratory *(Northgate Rd & South Cass Ave)*
**1:15 PM – 2:00 PM** – Security clearance and ID check at the main gate
(*REAL ID or valid passport required*)
**2:00 PM – 2:15 PM** – Arrive at APS, divide into groups, meet guides

**2:15 PM – 2:30 PM** – Welcome remarks by Jonathan Lang and Stefan Vogt
**2:45 PM – 3:45 PM**
**4:00 PM – 5:00 PM**
**5:00 PM – 5:15 PM** – Load buses
**5:15 PM – 5:45 PM** – Return to The Westin Chicago Lombard

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**Please remember to bring your conference badge, government-issued ID, and any personal items you may need.**

**PS3: Poster Session #3**
5:30 - 7:30pm Monday, 21st July, 2025
Session Room: Exhibit Hall
Chairs Cora Lind-Kovacs, Tim Stachowski, Leighanne Gallington
Join us at one (or all!) of our three engaging poster sessions during ACA2025! These sessions offer a fantastic opportunity to explore cutting-edge research, connect directly with authors, and dive into thought-provoking discussions across a wide range of crystallographic topics. Whether you're a seasoned scientist or a first-time attendee, poster sessions are a great way to engage with the community, ask questions, and discover new ideas. Don't miss the chance to be inspired by the incredible work being shared—check the schedule and make time to stop by!

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**18 Selenium-derivatized Nucleic Acids for Phasing, Crystal Growth, Structure Determination and Beyond**
Prof. Zhen Huang Ph.D.[1], Hehua Liu Ph.D.[1], Jianhua Gan Ph.D.[2]
[1]SeNA Research Institute, College of Life Sciences, Hubei University, Wuhan, Hubei, China. [2]School of Life Sciences, Fudan University, Shanghai, Shanghai, China

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**69 Structures of 1-deoxy-D-xylulose 5-phosphate (DXP) Reductoisomerase (IspC) from *Acinetobacter baumannii* in complex with Potential Inhibitors for Antimicrobial Drug Development**
Meagan Belcher Dufrisne PhD[1], Misgina Girma[2], Kyung Hyeon Lee PhD[2], Soo Hyeon Lee[1], Iswarduth Soojhawon PhD[1], Robin Couch PhD[2], Cynthia Dowd PhD[3], Schroeder Noble PhD[1]
[1]Walter Reed Army Institute of Research, Silver Spring, MD, USA. [2]George Mason University, Department of Chemistry and Biochemistry, Manassas, VA, USA. [3]George Washington University, Department of Chemistry, Washington DC, Washington DC, USA

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**71 A Novel Barium Complex of a Phenoxazinone Sulfonate Dye**
Philip J Squattrito[1], Jared T. Doney[1], Christopher G. Gianopoulos[2]
[1]Central Michigan University, Mount Pleasant, Michigan, USA. [2]University of Toledo, Toledo, Ohio, USA

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**79 STARS: Creating robust infrastructure to scale up structural biology programs for students**
Susanna Huang
Georgia Institute of Technology, Atlanta, GA, USA. Structural Nucleic Acid Anticancer Research Society (STARS), Atlanta, Georgia, USA

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**99 From 2-acetyl-indan-1,3-dione to 2*H*-1,5-benzodiazepines and their versatile applied features**

Prof. Gordana Pavlović PhD[1], Prof. Anife Ahmedova PhD[2], Prof. Marin Marinov[3]
[1]University of Zagreb Faculty of Textile Technology, Zagreb, Grad Zagreb, Croatia. [2]Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Sofia, Bulgaria. [3]Agricultural University – Plovdiv, Department of Chemistry and Phytopharmacy, Faculty of Plant Protection and Agroecology, Plovdiv, Plovdiv, Bulgaria

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**115 Current Status of the Liquid-Metal-Jet X-ray Source Technology**

Dr Camilla Storaa PhD, Dr Björn A. M. Hansson PhD, Dr Mikael Otendal PhD, Martin Norrefeldt MSc
Excillum, Kista, MN, Sweden

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**143 Visualizing Biological Systems at the Molecular and Cellular Level at the Laboratory for BioMolecular Structure**

Liguo Wang PhD, Guobin Hu PhD, Jake Kaminsky, Qun Liu PhD, Sean McSweeney PhD
Brookhaven National Laboratory, Upton, NY, USA

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**145 Updated Search for Alternative Unit Cells**

Dr Herbert J Bernstein PhD[1], Dr Lawrence C Andrews PhD[2]
[1]Fresh Pond Research Institute, Cambridge, MA, USA. [2]Ronin Institute for Independent Scholarship, Kirkland, WA, USA

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**151 Unit Cells in Space or Spaces for Unit Cells**

Dr. Lawrence C Andrews PhD[1], Dr. Herbert J Bernstein PhD[2]
[1]Ronin Institute for Independent Scholarship, Kirkland, WA, USA. [2]Fresh Pond Research Research Institute, Cambridge, MA, USA

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**164 How protein kinase inhibitors bind to the hinge region of the target protein.**

Assistant Professor Urszula Derewenda PhD[1], Professor Steve Scheiner PhD[2], Professor Zygmunt S Derewenda PhD[1]
[1]University of Virginia, Charlottesville, Virginia, USA. [2]State University of Utah, Logan, Utah, USA

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**166 Structural and functional impact of MPro$^{G48Y/\Delta P168}$ mutations in SARS-CoV-2 main protease exhibiting resistance to potent inhibitors**

Dr. Dipendra Bhandari PhD[1], Dr. Oksana Gerlits PhD[2], Dr. Stephen Keable PhD[1], Dr. Leighton Coates PhD[1], Dr. Annie Aniana PhD[3], Dr. Rodolfo Ghirlando PhD[3], Dr. Nashaat Nashed PhD[3], Dr. Andrey Kovalevsky PhD[1], Dr. John Louis PhD[3]
[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [2]Tennessee Wesleyan University, Athens, Tennessee, USA. [3]National Institutes of Health, Bethesda, Maryland, USA

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**167 Automated Cryo-EM Processing of GPCRs in CryoSPARC**

Kye Stachowski PhD
Structura Biotechnology, Toronto, Ontario, Canada

**176 RCSB Protein Data Bank (PDB): Driving Research and Education Using Experimentally-Determined Structures and Computed Structure Models from Artificial Intelligence/Machine Learning**

Dr. Yuhe Liang, Christine Zardecki, RCSB PDB Team
RCSB Protein Data Bank (PDB), Piscataway, NJ, USA

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**180 Using the Quantum Interface in Phenix to improve and automate metal coordination in macromolecular models**

Dr Nigel W Moriarty PhD
LBL, Berkeley, CA, USA

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**289 *How Experimental Adjustments and Optimizations led to Success in obtaining Enzyme-Ligand Crystal Structures of Zymoseptoria tritici ACCase Carboxyltransferase domain***

Dr. Timothy J. Rydel Ph.D.[1], Dr. Rachappa Balkunde Ph.D.[1], Mr. Timothy Boyle B.S.[1], Dr. Rong Ma Ph.D.[1], Dr. Paramita Deria Ph.D.[1], Dr. Michael Crawford Ph.D.[1], Dr. Virginie Lempereur Ph.D.[2], Dr. Tommi White Ph.D.[1]
[1]Bayer Research and Development Services LLC, Chesterfield, MO, USA. [2]Bayer S.A.S., La Dargoire, FRANCE, France

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**442 Characterization of Small Molecule Inhibition of Avian Influenza Hemagglutinin**

Amir Shimon Ph.D.
UIC, Chicago, IL, USA

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**264 RNAprecis: Prediction of full-detail RNA conformation from the experimentally best-observed sparse parameters**

Christopher J Williams[1], Henrik Wiechers[2], Benjamin Eltzner[2], Jane S Richardson[1], Stephan F Huckemann[2]
[1]Duke University, Durham, NC, USA. [2]University of Göttingen, Göttingen, Lower Saxony, Germany

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**223 Advances in cryo-electron microscopy (cryoEM) and X-Ray for structure-based drug discovery**

Pawel Rubach Ph.D.[1,2], Wladek Minor Ph.D.[1]
[1]University of Virginia, Charlottesville, VA, USA. [2]Warsaw School of Economics, Warsaw, Mazowieckie, Poland

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**188 Time-Resolved Pump-Probe X-Ray Solution Scattering Capabilities at BioCARS 14 ID Beamline, Advanced Photon Source.**

Dr. Irina Kosheleva Ph.D., Dr. Robert Henning Ph.D., Dr. Insik Kim Ph.D., Mr. Eric Zoellner B.S., Professor Vukica Srajer Ph.D., Professor Rama Ranganathan Ph.D.
The University of Chicago, Chicago, IL, USA

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**269 User-Friendly Continuous Serial Electron Diffraction Data Processing**

Paul Hager, Gerhard Hofer, Lei Wang, Laura Pacoste, Alexis Fonjallaz, Xiaodong Zou

Stockholm University, Stockholm, Stocholms län, Sweden

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**462 Revolutionizing Small Molecule Drug Discovery Pipelines with Cryo-EM: A Workflow for High-Throughput Screening and High-Resolution Data Collection**

Adrian F Koh[1], Victoria Cushing[2], Basil Greber[2], Pascal Lill[3], Surajit Banerjee[3], Zuben Brown[3], Abhay Kotecha[1]

[1]Thermo Fisher Scientific, Eindhoven, North Brabant, Netherlands. [2]The Institute of Cancer Research, Sutton, London, United Kingdom. [3]Thermo Fisher Scientific, Portland, Oregon, USA

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**454 Cryo-EM structures of the immunodominant chlamydial antigen Major Outer Membrane Protein (MOMP) and its complex with a conformational neutralizing monoclonal antibody**

Yirui Guo[1,2], Megan Shelby[3], Patrik D'haeseleer[3], Sukumar Pal[4], Anatoli Slepenkin[4], Beverly Robinson[3], Zbyszek Otwinowski[1], Brent Segelke[3], Matthew Coleman[3,5], Dominika Borek[1], Luis de la Maza[4]

[1]UT Southwestern, Dallas, TX, USA. [2]Ligo Analytics, Dallas, TX, USA. [3]Lawrence Livermore National Laboratory, Livermore, CA, USA. [4]UC Irvine, Irvine, CA, USA. [5]UC Davis, Sacramento, CA, USA

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

Robert Henning, Vukica Srajer, Irina Kosheleva, Insik Kim, Eric Zoellner, Rama Ranganathan

The University of Chicago, Chicago, IL, USA

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**357 RAPD2: Rapid Automated Processing of Macromolecular Crystallographic Data 2**

Jonathan P Schuermann Ph. D., Kay Perry Ph. D., David Neau Ph. D., Frank V. Murphy Ph. D.

Cornell University, Ithica, NY, USA

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**372 Conformational alterations in the protein-DNA complex facilitates efficient integration of diverse DNA substrates by the CRISPR Cas1-Cas2 proteins**

Alberto Monteiro Dos Santos, Saadi Rostami, Richard Van, Kole Long, Swarmistha Devi Aribam, Yihan Shao, Rakhi Rajan

University of Oklahoma, Norman, OK, USA

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**477 Metal-Organic Frameworks (MOFs) Based Heterojunction for the Photocatalytic Degradation of PFAS**

Adarsh Nayarassery Narayanan

University of Texas at Dallas, Richardson, TX, USA

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**493 Structural and biochemical characterization of arabinose nucleosides as inhibitors of the SARS-CoV-2 polymerase**

Ziyang Xiao, Thomas K. Anderson, Robert N. Kirchdoerfer

University of Wisconsin Madison, Madison, WI, USA

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**495 Structural insights into the mechanism of malaria-protective antibodies from the IGHV3-49/IGKV2D-29 lineage**

Dr. Monika Jain Ph.D.[1], Dr. Ian A. Wilson Ph.D.[1,2]
[1]The Scripps Research Institute, La Jolla, California, USA. [2]The Skaggs Institute for Chemical Biology, La Jolla, California, USA

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**506 SER-CAT Studies: Implications to Dose Reduction by MDS (Multiple-DataSet) Data Collection Strategy**

Unmesh Chinte Ph.D., Zheng-Qing (Albert) Fu Ph.D., Zhongmin Jin Ph.D., John Rose Ph.D., John Chrzas Ph.D., Bi-Cheng Wang Ph.D.
SER-CAT and University of Georgia, Athens, GA, USA

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**505 Recent Developments at SSRL BL4-2, a Beamline for Biological Small and Wide Angle X-ray Scattering**

Dr Thomas M Weiss PhD
SSRL, Menlo Park, CA, USA

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**508 *Burkholderia pseudomallei* rubrerythrin binds metals promiscuously in a pre-formed four-helix bundle**

Gabrielle R. Budziszewski PhD[1,2], Dr. Miranda L. Lynch PhD[1,3], M. Elizabeth Snell MS[1,2], Dr. Diana C.F. Monteiro PhD[4], Dr. Sarah E.J. Bowman PhD[1,2]
[1]University at Buffalo-Hauptman Woodward Research Institute, Buffalo, NY, USA. [2]University at Buffalo, Jacobs School of Medicine, Department of Biochemistry, Buffalo, NY, USA. [3]University at Buffalo, Jacobs School of Medicine, Department of Structural Biology, Buffalo, NY, USA. [4]Center for Structural Biology, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Frederick, MD, USA

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**509 Advancing Structure-Based Drug Development: A Rebuild of the IMCA-CAT Beamline at the Advanced Photon Source**

Melissa Carrillo PhD[1], John P. Bacik PhD[1], Erica Duguid PhD[1], J. Lewis Muir[1], Clark Williams[1], Andrew Mayton[1], Kevin D'Amico PhD[2], Stephan Ginell PhD[3], Nathan Brown[4], Lisa J. Keefe PhD[1]
[1]Industrial Macromolecular Crystallography Association Collaborative Access Team (IMC-CAT) Sector 17-ID, Lemont, IL, USA. [2]137partners, LLC, Bridgton, ME, USA. [3]Consultant, Naperville, IL, USA. [4]AIM Concepts, Littleton, CO, USA

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**499 Crystallographic Analysis of the Storage Protein Tub – a Tungstate Binding Protein from *Eubacterium limosum***

Dr. Dayong Zhou PhD, Dr. John P Rose PhD, Dr. Nana Shao PhD, Dr. Lirong Chen PhD, Dr. Gerrit J. Schut PhD, Farris L Poole MS, Dr. Michael W. W. Adams PhD, Dr. B.C. Wang PhD
University of Georgia, Athens, GA, USA

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**517 CryoEM structures of evolved Family B DNA polymerase bound to template-primer substrates**

Millie M. Georgiadis PhD[1], Nicole Leal PhD[2], Steven A. Benner PhD[2]
[1]Indiana University School of Medicine, Indianapolis, IN, USA. [2]Foundation for Applied Molecular Evolution, Alachua, Florida, USA

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**518 Dihydroorotase from *Methanococcus jannaschii* with substrate bound**
Dr. Jacqueline Vitali Ph.D.[1], Dr. Jay C. Nix Ph.D.[2], Ms. Haley E. Newman B.S.[1], Dr. Michael J. Colaneri Ph.D.[3]
[1]Cleveland State University, Cleveland, OH, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [3]SUNY at Old Westbury, Old Westbury, NY, USA

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**519 Removal of Per- and Polyfluoroalkyl Substances from Contaminated Groundwater using Cationic Metal−Organic Frameworks**
Arefeh Mirsharifian, Dr. Mario Wriedt
University of Texas at Dallas, Richardson, Texas, USA

**All Members Business Meeting**
7:30 - 8:15pm Monday, 21st July, 2025
Session Room: Junior Ballroom C

**SIG Mixer**
8:15 - 9:15pm Monday, 21st July, 2025
Session Room: Junior Ballroom B

**Registration Desk**
7:30 - 11:00am Tuesday, 22nd July, 2025
Session Room: Grand Ballroom Foyer

**4.1.2 Structure of Nucleic Acids**
8:30 - 11:30am Tuesday, 22nd July, 2025
Session Room: Lilac AC
Chairs Peter Hsu, 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.

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8:30 - 9:00am
**179 The Art of Chromosome Capture: Kinetochore Structures Across Evolution.**
Dr Stanislau Yatskevich
Genentech, South San Francisco, CA, USA

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9:00 - 9:30am
**111 Cryo-EM Studies of Genome Organization and Transcription Complexes**
Seychelle M Vos PhD
Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

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9:30 - 10:00am
**212 Structural basis of LARP1-mediated regulation of TOP mRNA via the 40S small ribosomal subunit**

Wenzhao Dong[1,2], Mario R. Blanco[3], Ross Kaufhold[1,2], Erica Wolin[4], Jimmy K. Guo[3], Marko Jovanovic[4], Mitchell Guttman[3], Jailson Brito Querido[1,2]
[1]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI, USA. [2]Life Sciences Institute, University of Michigan, Ann Arbor, MI, USA. [3]Division of Biology and Bioengineering, California Institute of Technology, Pasadena, CA, USA. [4]Department of Biological Sciences, Columbia University, New York, NY, USA

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10:30 - 10:50am
**224 A Cryo-EM Method to Solve Small Nucleic Acid Structures**
Holly L. Shultz, Evan R. Cramer, Aaron R. Robart Ph.D.
West Virginia University, Morgantown, West Virginia, USA

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10:50 - 11:10am
**378 Complex Water Networks Visualized through Cryogenic Electron Microscopy of RNA**
Rachael C Kretsch[1], Shanshan Li[2], Grigore Pintilie[1], Michael Z Palo[1], David A Case[3], Rhiju Das[1], Kaming Zhang[2], Wah Chiu[1]
[1]Stanford University, Palo Alto, CA, USA. [2]University of Science and Technology of China, Hefei, N/A, China. [3]Rutgers University, Piscataway, NJ, USA

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11:10 - 11:30am
**291 Cryo-EM Structures of Group II Intron Ribonucleoprotein Complexes**
Sarah A Starcovic, Evan R Cramer, Dr. Aaron R Robart Ph.D.
West Virginia University, Morgantown, WV, USA

### 4.1.3 Ab initio Designed Proteins

8:30 - 11:30am Tuesday, 22nd July, 2025
Session Room: Magnolia A
Chairs Vardhan Satalkar, Jack Nicoludis
New advancements in machine learning have recently and remarkably improved our ability to predict and design proteins. This session will explore the exciting field of protein design, where computational and experimental methods combine to engineer proteins with tailored structures and functions. A wide variety of topics will be covered, such as advancements in AI/ML methods in protein structure prediction and design, directed evolution and rational design, structural characterization of designed proteins, and applications of protein design, such as in synthetic biology, biomedical imaging, and drug discovery. The program is designed to address not only the technical challenges associated with protein design but also to enhance understanding of the relationship between protein structure, function, and dynamics, thereby expanding their range of applications in translational research.

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8:30 - 9:00am
**76 Harnessing Conformational Dynamics and Computational Design to Generate Novel Enzymes**
Prof. Lynn Kamerlin PhD
Georgia Institute of Technology, Atlanta, GA, USA

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9:00 - 9:30am

**148 How dynamics in hydrogen-bonding networks define proton channel selectivity and conductivity**
Huong T. Kratochvil PhD, Nolan Jacob, Vincent Silverman, Gisselle Prida Ajo
UNC-Chapel Hill, Chapel Hill, NC, USA

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9:30 - 10:00am
**238 Applications and properties of computationally designed *de novo* proteins**
Martin Pacesa PhD
EPFL, Lausanne, Vaud, Switzerland

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10:30 - 11:00am
**254 Peptide Frameworks as Microcosms of Metalloproteins**
Prof Andy I Nguyen Ph.D.
University of Illinois Chicago, Chicago, IL, USA

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11:00 - 11:30am
**421 Machine Learning Protein Motif Fusion for Avid Sensing, Intracellular Reporters, and Crystalline Assemblies**
Ethan T Shields, Emma N Magna, Callie K Slaughter, Pegah Eizadkhah, Christopher D Snow
Colorado State University, Fort Collins, CO, USA

**4.1.4 Cool Structures**
8:30 - 11:30am Tuesday, 22nd July, 2025
Session Room: Lilac D
Chairs Nichole Valdez, Kamran Ghiassi

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8:35 - 9:00am
**157 Investigating Macrolactone Formation by Thioesterase Domains through Incorporation of an Unnatural Amino Acid**
Vishakha Choudhary, Tyler M. McCullough Ph.D, Janet L. Smith Ph.D.
University of Michigan, Ann Arbor, MI, USA

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9:00 - 9:30am
**276 Single-Crystal to single-crystal copolymerization in a $Pt(acac)_2$•TCNQ cocrystal with new TCNQ reactivity and coordination mode**
Prof. Larry R. Falvello Ph.D.[1,2,3], Dr. Miguel Baya Ph.D.[4,3], Dr. Slavomira Šterbinská[1,2,3], Dr. Milagros Tomás Ph.D.[4], Dr. Esteban P. Urriolabeitia Ph.D.[4]
[1]CSIC-University of Zaragoza, Zaragoza, Aragón, Spain. [2]Aragón Nanoscience and Materials Institute, Zaragoza, Aragón, Spain. [3]Dept. of Inorganic Chemistry, Zaragoza, Aragón, Spain. [4]Instituto de Síntesis Química y Catálisis Homogénea, CSIC-University of Zaragoza, Zaragoza, Aragón, Spain

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9:30 - 10:00am
**13 Dual Substrate Binding stabilizes the Catalytic State in Ketohexokinase**
So Young Bae PhD Student, Karen N. Allen, Dean R. Tolan
Boston University, Boston, MA, USA

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10:30 - 11:00am
**138 From Skeptic to Believer: Monitoring a Ring-Opening Isomerization of a CeIV Complex in the Solid-State Using a Home-Source Diffractometer**
Michael Gau
University of Pennsylvania, Philadelphia, PA, USA

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11:00 - 11:30am
**41 Structure of TnsABCD transpososome reveals mechanisms of targeted DNA transposition**
Shukun Wang[1], Romana Siddique[1], Mark Hall[1], Phoebe Rice[2], Leifu Chang[1]
[1]Purdue University, West Lafayette, Indiana, USA. [2]The University of Chicago, Chicago, Illinois, USA

**4.1.5 Cryo-EM facilities: How to integrate multiple modalities on one instrument**
8:30 - 11:30am Tuesday, 22nd July, 2025
Session Room: Magnolia BC
Chairs Tamir Gonen, Brent Nannenga
The use of cryo-EM is expanding with several techniques including single particle cryo-EM, MicroED, and cryo-electron tomography using the same instrumentation. Many institutions are adding these technique to their suite of structure determination methods.This session will focus on experiences integrating and applying the different modalities of cryo-EM, and the best practices to ensure that all cryo-EM methods can coexist.

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8:35 - 8:55am
**375 Challenges and Insights into integrating Single-Particle Cryo-EM and MicroED**
Ampon C Saeher PhD, Tamir Gonen
UCLA, Los Angeles, CA, USA

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8:55 - 9:15am
**90 Integrative Approaches in Structural Science: Bridging Electron and X-ray Techniques**
Brandon Q. Mercado
Yale University, New Haven, Connecticut, USA

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9:15 - 9:35am
**227 Keeping 3D electron crystallography relevant: Leveraging new technologies for 3D ED/MicroED at a regional cryoEM center**
M. Jason de la Cruz
Structural Biology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY, USA. Cryo-Electron Microscopy Innovation Laboratory, Memorial Sloan Kettering Cancer Center, New York, NY, USA

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9:35 - 10:00am
**53 Integrating MicroED into an X-ray Facility: Enjoying the Journey and Expanding Your Horizons**
Joseph D Ferrara PhD
Rigaku Americas, The Woodlands, TX, USA

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10:30 - 10:50am
**4 Making MicroED Accessible at a CryoEM Center Through Training and Infrastructure**
Edward T Eng[1], Christina Zimanyi[1], Daniel Decato[2], Jessalyn G Miller[1], Chun-Hsing Chen[3]
[1]New York Structural Biology Center, New York, NY, USA. [2]University of Montana, Missoula, MT, USA. [3]University of North Carolina at Chapel Hill, Chapel Hill, NC, USA

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10:50 - 11:10am
**356 Accelerating drug discovery at Exelixis through cryo-EM**
William J Nicolas PhD
Exelixis, Alameda, CA, USA

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11:10 - 11:30am
**283 Pipe(line) dreams for MicroED/3DED sample preparation**
Katherine A Spoth[1,2], Gabrielle R Budziszewski[1,3], M Elizabeth Snell[1,3], Miranda L Lynch[1,2], Devrim Acehan[1,2], Sarah EJ Bowman[1,3]
[1]UB HWI, Buffalo, NY, USA. [2]University at Buffalo, Jacobs School of Medicine and Biomedical Science, Department of Structural Biology, Buffalo, NY, USA. [3]University at Buffalo, Jacobs School of Medicine and Biomedical Science, Department of Biochemistry, Buffalo, NY, USA

**4.1.6 Fibers and Friends: X-ray Vision for Unmasking the Culprits in Neurodegenerative Disease**
8:30 - 11:30am Tuesday, 22nd July, 2025
Session Room: Lilac B
Chairs Rama Sashank Madhurapantula, Joseph Orgel, Olga Antipova

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8:30 - 8:55am
**246 Paleontological Puzzles, Neurological Solutions: How Dinosaur Collagen Analysis Advanced X-ray Scanning for TBI**
Professor Joseph Orgel, Dr Rama Sashank Madhurapantula
Illinois Tech, Chicago, Il, USA

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8:55 - 9:15am
**249 Utilizing small-angle X-ray microdiffraction to explore neurodegeneration in human brain tissue**
Prakash Nepal PhD, Abdullah Al Bashit PhD, Lee Makowski PhD
Northeastern University, Boston, MA, USA

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9:15 - 9:35am
**358 Understanding the structural characteristics of macromolecular assemblies in connective tissues.**
Dr. Olga Antipova PhD[1], Dr. Joseph Orgel PhD[2], Dr Thomas Irving PhD[3], Dr Raul Barrea PhD[4]
[1]Argonne National Laboratory, Lemont, IL, USA. [2]Illinois Institute of Technology, Chicago, IL, USA. [3]Illinois Institute ofTechnology, Chicago, IL, USA. [4]DePaul University, Chicago, IL, USA

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9:35 - 10:00am
**97 Functionality of the mineralized cartilage of shark vertebral centra**

Dr. Stuart R. Stock PhD[1], Dr. Jason T Parker PhD[2], Mr. Jackson - Comes B.S.[3], Dr. Jong - Seto PhD[3], Dr. Michelle S. Passerotti PhD[4], Dr. Lisa J. Natanson PhD[5], Dr. Dilworth Y. Parkinson PhD[2], Dr. Jun S. Park PhD[6]
[1]Northwestern University, Chicago, IL, USA. [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [3]Arizona State University, Tempe, AZ, USA. [4]National Marine Fisheries Service, NOAA, Narragansett, RI, USA. [5]Independent Scientist, Homer, AK, USA. [6]Advanced Photon Source, Argonne National Laboratory, Lemont, IL, USA

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10:30 - 10:50am

**133 Development of Pty-co-SAXS: Combined Ptychography and Small-Angle X-ray Scattering at APS 12-ID-E**

Dr. Byeongdu Lee, Dr. Soenke Seifert, Dr. Joseph McCourt, Dr. Junjing Deng
Argonne National Laboratory, Lemont, IL, USA

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10:50 - 11:10am

**351 Multi-modal imaging using scanning diffraction and microscopy to elucidate tissue architecture**

Rama S. Madhurapantula
Illinois Institute of Technology, Chicago, IL, USA

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11:10 - 11:30am

**330 New Capabilities of the MuscleX Data Reduction Package for Fiber Diffraction from Muscle and other Fibrous Systems.**

Dr. Thomas C Irving Ph.D>
Illinois Insitute Of Technology, Chicago, Illinois, USA

**PL4 Trueblood Award: Professors Branton J. Campbell & Harold T. Stokes**

11:45am - 12:45pm Tuesday, 22nd July, 2025
Session Room: Junior Ballroom C

Professors Branton J. Campbell and Harold T. Stokes of Brigham Young University have been named recipients of the Robert Bau Neutron Diffraction Award. This award honors outstanding accomplishments in the field of neutron diffraction and commemorates the legacy of Professor Robert Bau's impact on structural science.

Together, Professors Campbell and Stokes have made foundational contributions to the use of symmetry-mode analysis in interpreting neutron diffraction data. Their development of the ISOTROPY Software Suite, including tools like ISODISTORT and FINDSYM, has transformed how crystallographers characterize structural phase transitions — particularly in complex magnetic and functional materials.

Dr. Campbell's research integrates neutron powder and single-crystal diffraction techniques to explore structure-property relationships, while Dr. Stokes has led the crystallographic community in developing group-theoretical methods essential to symmetry analysis. Their decades-long collaboration has empowered researchers worldwide through accessible, rigorous computational tools and has advanced standards in magnetic structure communication.

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**353 New directions and opportunities for symmetry-centric structural science**

Branton J. Campbell, Harold T. Stokes

Brigham Young University, Provo, Utah, USA

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**382 New directions and opportunities for symmetry-centric structural science**
Harold T Stokes, Branton Campbell
Brigham Young University, Provo, UT, USA

**DEI-3A #IAmRemarkable - PREREGISTRATION REQUIRED**
12:45 - 1:55pm Tuesday, 22nd July, 2025
Session Room: Cypress A
Chairs Alexis Davidson, Alice Thwin, Sandra Gabelli
#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

**DEI-3B #IAmRemarkable - PREREGISTRATION REQUIRED**
12:45 - 1:55pm Tuesday, 22nd July, 2025
Session Room: Cypress B
Chairs Alexis Davidson, Alice Thwin, Sandra Gabelli
#IAmRemarkable is an initiative empowering women and other underrepresented groups to celebrate their achievements in the workplace and beyond. Its goal is to improve 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 lives.

**Career Odysseys/Career Panel**
12:45 - 1:45pm Tuesday, 22nd July, 2025
Session Room: Magnolia A
Chairs Edward Pryor, Melanie Adams-Cioaba

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**103 Career Odysseys panel - Chrencik**
Jill Chrencik PhD
Merck, South San Francisco, CA, USA

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**113 Grad student to biotech to pharma: career odyssey of an industrial structural biologist**
David M Dranow Master's Degree
UCB, Bainbridge Island, WA, USA

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**373 North, North, North and the border between academia and research institutions**
Dr. Vivian Stojanoff PhD
National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA

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**380 Is a career in industry for you?**
Dr Pamela A Williams DPhil
Astex Pharmaceuticals, Cambridge, Cambs, United Kingdom

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**400 Life in a University Crystallography Service Facility**
Carla Slebodnick
Virginia Tech, Blacksburg, VA, USA

**4.2.1 AI/ML in Modern Structural Science**
2:00 - 5:00pm Tuesday, 22nd July, 2025
Session Room: Junior Ballroom C
Chairs Debanu Das, Emre Brookes, Daniel Olds
The rapid advancements in artificial intelligence (AI) and machine learning (ML) are revolutionizing various scientific domains, including materials science, chemistry, physics, biology, and others. This session aims to explore how AI and ML techniques can be utilized in structural science in applications ranging from data analysis, structure determination, structure-based drug discovery and materials characterization to facility operation and sample throughput.
Submissions from all areas of structural science are welcome and could discuss challenges in AI/ML integration, present novel algorithms, or offer solutions for specific situations. Part 1 will focus on AI/ML applications to materials systems while Part 2 will focus on AI/ML applications to biological systems.

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2:00 - 2:30pm
**177 CrystalPilot: A machine-learning based software platform for single crystal neutron diffraction experiments**
Zhongcan Xiao, Guannan Zhang, Zachary Morgan, Viktor Reshniak, Xiaoping Wang
Oak Ridge National Laboratory, Oak Ridge, TN, USA

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2:30 - 3:00pm
**342 The Sol platform: Integrating computation and ML/AI with structural data for research and drug discovery**
Dr. Seth F. Harris PhD
Genentech, South San Francisco, CA, USA

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3:30 - 4:00pm
**64 NucleoFind: A Deep-Learning Network for Interpreting Nucleic Acid Electron Density**
Jordan S Dialpuri, Jon Agirre, Kathryn D Cowtan, Paul D Bond
University of York, York, North Yorkshire, United Kingdom

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4:00 - 4:30pm
**282 Machine-learning and structure-based discovery of SARS-CoV-2 papain-like protease ($PL^{pro}$) inhibitors with efficacy in a murine infection model**
Dr. Ellene H. Mashalidis PhD

Pfizer, Groton, CT, USA

**4.2.2 Small Molecule Crystal Structures for Pharmaceutical Development**
2:00 - 5:00pm Tuesday, 22nd July, 2025
Session Room: Lilac AC
Chairs Luca Iuzzolino, Justin Newman
Understanding the various properties of active pharmaceutical ingredients (APIs), including but not limited to physical, chemical, thermodynamic, kinetic, spectroscopic, mechanical, and surface properties, is of utmost importance to ensure a robust and reliable manufacture of small molecule drug products. This session aims to explore the ways that structure elucidation can impact our understanding of solid state properties and how they influence the manufacture of a robust drug product. Potential topics for this session could include drug substance form selection, properties (chemical or physical), polymorphism, and how these can potentially impact the design of a final drug product.

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2:00 - 2:30pm
**183 Prediction of solid-to-solid phase transition for risk assessment of solid forms using quantum mechanical solid-state computations**
Satish Iyemperumal, Charlene Tsay, Monika Warzecha, Ales Medek, Kevin Gagnon, Jiahui Chen
Vertex Pharmaceuticals Inc., Boston, MA, USA

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2:30 - 3:00pm
**369 MicroED and its Impact on Form Space Elucidation**
Principal Scientist Roger D Sommer PhD
Bristol Myers Squibb, New Brunswick, NJ, USA

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3:30 - 4:00pm
**371 Solid-State Form Design in Pharmaceutical Drug Product Development**
Dr. Rajni Miglani Bhardwaj
Pfizer, Groton, CT, USA

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4:00 - 4:30pm
**20 How crystal structure prediction can impact small-molecule pharmaceutical development: past examples, success stories, and future prospects.**
Luca Iuzzolino
Merck & Co. Inc., Rahway, NJ, USA

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4:30 - 5:00pm
**95 Resistance Fighters: Developing a Novel HMG-CoA Reductase Inhibitor to Combat Gram-Positive Bacteria**
Dr. Phillip S Rushton PhD[1], Dr. Calvin N Steussy MD, PhD[1], Dr. Sucharita Bose PhD[2], Dr. Daneli Lopez-Perez PhD[3], Mr. Tim Schmidt bachelors[1], Dr. Mohamed N Seleem DVM, MS, PhD[4], Dr. Mark Lipton PhD[1], Dr. Cynthia V Stauffacher PhD[1]
[1]Purdue University, West Lafayette, IN, USA. [2]Institute for Stem Cell Science and Regenerative Medicine (DBT-inStem), Bengalore, Karnataka, India. [3]Food and Drug Administration, Silver Springs, MD, USA. [4]Virginia Tech, Blacksburg, VA, USA

**4.2.3 Engaging Students with Crystallography**
2:00 - 5:00pm Tuesday, 22nd July, 2025
Session Room: Magnolia A
Chairs Susanna Huang, Yinka Olatunji-Ojo, Joe Tanski
This session is focused on how to effectively engage students at any level with crystallography in teaching, outreach and research. Specific topics may include student training and mentoring, pedagogy and building crystallography teaching infrastructure, strategies for faculty professional success in research involving crystallography, effective involvement of students at synchrotron facilities, outreach programs to attract the interest of students to crystallography and structural biology, approaches towards instrument acquisition and maintaining resources for engaging students with crystallography.

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2:10 - 2:35pm
**14 Resolving Space-Group-Choice Dilemma in Small-Molecule Crystallography Education: A Case Study Approach**
Shao-Liang Zheng
Harvard University, Cambridge, MA, USA

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2:35 - 3:00pm
**245 Making X-ray crystallographic refinement accessible for non structural biologists**
Dr. Miki Senda PhD, Prof. Toshiya Senda PhD
KEK, Tsukuba, Ibaraki, Japan

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3:30 - 3:55pm
**361 Crystallizing Student-Interest in Biochemistry**
Ms. Selina S Huang[1,2], Ms. Susanna S Huang[1,2]
[1]STARS research society, Marietta, Georgia, USA. [2]Georgia Institute of Technology, Atlanta, Georgia, USA

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3:55 - 4:20pm
**316 STARS: Spread the beauty of DNA Crystallography**
Chenyi Andrew, Susanna Huang
Georgia Institute of Technology, Atlanta, Georgia, USA

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4:20 - 4:45pm
**368 Lessons Learned Implementing a Protein Crystallography CURE**
Krystle J McLaughlin PhD
Vassar College, Poughkeepsie, NY, USA

**4.2.4 MicroED for Macromolecules and Drug Discovery**
2:00 - 5:00pm Tuesday, 22nd July, 2025
Session Room: Magnolia BC
Chairs Johan Hattne, Mike Martynowycz
Building on the interplay between cutting-edge electron microscopy and minuscule crystal sizes, Microcrystal Electron Diffraction (MicroED) has become an indispensable tool for high-resolution structure determination of biological macromolecules and drug discovery. This session delves into unveiling newly determined macromolecular and new pharmaceutical structures facilitated

by MicroED. 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 and drug discovery.

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2:00 - 2:20pm

**93 A comparison of an electron diffraction and an X-ray diffraction experiment from a single protein microcrystal lamella**

Dr Adam D Crawshaw PhD[1], Dr David Owen PhD[1], Miss Melissa R Whyte-Fink BSc[2], Dr Anna J Warren PhD[1], Dr Pedro Nunes PhD[1], Dr Jose Trincao PhD[1], Dr Alistair Siebert PhD[1], Dr Gwyndaf Evans PhD[1,3]

[1]Diamond Light Source, Didcot, Oxfordshire, United Kingdom. [2]University of St. Andrews, St Andrews, Fife, United Kingdom. [3]Rosalind Franklin Institute, Didcot, Oxfordshire, United Kingdom

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2:20 - 2:40pm

**77 Measurement of chemical information using 3D ED and Cryo-EM**

Prof. Koji Yonekura Ph.D.

RIKEN, Sayo, Hyogo, Japan. Tohoku University, Sendai, Miyagi, Japan

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2:40 - 3:00pm

**273 Peak Performance: Advances in Macromolecular MicroED Data Collection**

Max T.B. Clabbers

Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Mid-Jutland, Denmark. Department of Molecular Biology and Genetics, Aarhus, Mid-Jutland, Denmark

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3:03 - 3:50pm

**263 Structural basis of signalling by TIR domain containing proteins**

Thomas Ve

Institute for Biomedicine and Glycomics, Griffith University, Goldcoast, QLD, Australia

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3:50 - 4:10pm

**328 Leveraging MicroED to determine structures of protein-bound synthetic small molecules and natural products**

Jose A Rodriguez

UCLA, Los Angeles, CA, USA

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4:10 - 4:30pm

**354 Development and application of new methods in micro-crystal Electron Diffraction (microED)**

William J Nicolas PhD

Exelixis, Alameda, CA, USA

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4:20 - 4:40pm

**313 MicroED beyond the traditional drug space**

Emma Danelius[1], Guanhong Bu[1], Tamir Gonen[2]

[1]UCR, Riverside, CA, USA. [2]UCLA, Los Angeles, CA, USA

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4:30 - 4:50pm
**194 Solving the native structures of protein nanocrystals grown in bacteria by electron diffraction**
Dr Marcus Gallagher-Jones
The Rosalind Franklin Institute, Harwell, Oxfordshire, United Kingdom

**4.2.5 SAS In Integrative Structural Approaches**
2:00 - 5:00pm Tuesday, 22nd July, 2025
Session Room: Lilac D
Chairs Alexander Yarawsky, Robert Monsen
This session will showcase recent advancements in leveraging small-angle scattering (SAS) data in combination with orthogonal biophysical, biochemical, and computational methods to elucidate complex biological structures that are challenging for traditional approaches like X-ray diffraction, NMR, or cryo-EM. The examples will include, but are not limited to, studies on higher-order molecular assemblies, their structures, and dynamics. The focus will be on how these integrative models enhance our understanding of the spatio-temporal environment of the human cell.

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2:02 - 2:20pm
**54 Determining accurate conformational ensembles of intrinsically disordered proteins at atomic resolution**
Mr Kaushik Borthakur[1], Mr Thomas R Sisk[1], Mr Francesco P Panei[2], Dr Massimiliano Bonomi[2], Dr Paul J Robustelli[1]
[1]Dartmouth College, Hanover, NH, USA. [2]Institut Pasteur, Paris, Paris, France

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2:20 - 2:40pm
**244 Integrating SAXS/WAXS with Molecular Dynamics: RNA Nanoparticles as a Case Study at the Life Sciences X-ray Scattering Beamline (LIX), NSLS-II**
Dr James Byrnes PhD[1], Dr Kriti Chopra PhD[1], Dr. Kirill Afonin PhD[2], Dr. Lewis A Rolband PhD[2], Dr Joanna K Krueger PhD[2], Dr Hubertus JJ van Dam PhD[1], Leyla Danai[2], Damian Beasock[2]
[1]Brookhaven National Laboratory, Upton, NY, USA. [2]UNC Charlotte, Charlotte, NC, USA

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2:40 - 3:00pm
**228 Bridging Experiment and AI: SAXS-Driven Molecular Dynamics Refinement of Predicted Biomolecular Structures**
Kriti Chopra PhD[1], Lewis A Rolband PhD[2], James Byrnes PhD[1], Kirill A Afonin[2], Hubertus JJ van Dam PhD[3]
[1]Brookhaven National Laboratory, Upton, New York, USA. [2]University of North Carolina Charlotte, Charlotte, North Carolina, USA. [3]Universität Duisburg-Essen, Essen, Essen, Germany

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3:30 - 3:50pm
**78 An Integrated Structural Model of the Palladin-Actin Complex Using XL-MS, SAXS, NMR, and Docking Approaches**
Dr. Moriah R Beck PhD[1], Rachel A Sargent BS[1], David H Liu BS[1], Dr. Rahul Yadav PhD[2]
[1]Wichita State University, Wichita, KS, USA. [2]University of Arkansas-Ft. Smith, Fort Smith, AR, USA

3:55 - 4:20pm

**100 Solution conformational differences between conventional and CENP-A nucleosomes are accentuated by reversible deformation under high pressure**

Kushol Gupta[1], Nikolina Sekulic[2], Praveen Kumar Allu[1], Nicklas Sapp[1], Qingqiu Huang[3], Kathryn Sarachan[4], Mikkel Christensen[2], Reidar Lund[2], Susan Krueger[5], Joseph E Curtis[5], Richard E Gillilan[3], Gregory D Van Duyne[1], Ben E. Black[1]

[1]University of Pennsylvania, Philadelphia, PA, USA. [2]University of Oslo, Oslo, na, Norway. [3]Cornell High Energy Synchrotron Source, Cornell University, Ithaca, NY, USA. [4]Wilson College, Chambersburg, PA, USA. [5]Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, USA

4:20 - 4:40pm

**295 Structural and Functional Characterization of SOSTDC1**

Melissa M Gouge B.S., Gregory Gipson Ph.D., Chandramohan Kattamuri Ph.D., Thomas B. Thompson Ph.D.

University of Cincinnati, Cincinnati, Ohio, USA

4:40 - 5:00pm

**326 SAXS and Alphafold for mechanistic understanding of protein conformational switching.**

ANU ANU Ph.D. scholar

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

**4.2.6 Structural Characterizations of Emerging Energy Materials**

2:00 - 5:00pm Tuesday, 22nd July, 2025

Session Room: Lilac B

Chairs Hao Liu, Si Athena Chen

Structural characterizations of the next-generation energy materials are crucial for establishing precise relationships between chemistry, synthesis procedures, performance, and stability. This session invites works that apply in-depth structural characterizations on emerging energy materials for applications such as batteries, fuel cells, photovoltaics, thermoelectrics, piezoelectric devices, etc. Submissions may be steady-state or time-resolved structural studies of crystalline or amorphous energy materials, to understand the phase evolution during synthesis, structure-property relationships, degradation mechanisms, and other related aspects.

2:00 - 2:20pm

**72 Designing Sustainable Materials for Energy Applications**

Alicia M Manjon Sanz[1], Brooke Richtik[2], Abby Neill[3], Nabaraj Pokhrel[1], Mohit Chandra[1], Michelle R. Dolgos[1], Valentino Cooper[1]

[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. [2]University of Calgary, Calgary, Alberta, Canada. [3]Johns Hopkins University, Baltimore, Maryland, USA

2:20 - 2:40pm

**94 Design and Development of Solid Electrolyte Materials Inspired and Guided by In-depth Crystal Structure Characterizations**

Dr. Zhantao Liu[1], Dr. Jue Liu[2], Professor Yifei Mo[3], Professor Hailong Chen[1]

[1]Georgia Institute of Technology, Atlanta, GA, USA. [2]Oak Ridge National Lab, Oak Ridge, TN, USA. [3]University of Maryland, College Park, MD, USA

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2:40 - 3:00pm

**205 Time-resolved X-ray diffraction studies of mineral transformations in aqueous solutions**

Dong Youn Chung[1], Peter J. Heaney[1], Joanne E. Stubbs[2], Peter J. Eng[2]

[1]Pennsylvania State University, University Park, PA, USA. [2]The University of Chicago, Chicago, IL, USA

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3:30 - 3:50pm

**169 Structural Evolution during Chemical and Electrochemical Intercalation Reactions Probed with X-rays, Neutrons, and RF Pulses**

Sarah Ko, Prof. Kent J. Griffith

UC San Diego, San Diego, CA, USA

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3:50 - 4:05pm

**186 Neutron and X-ray Diffraction Investigation of Crystal Structure and Phase Transition for $Na_{2/3}[Ni_yMn_zAl_{1-y-z}]O_2$ as a Cathode Material for Sodium-ion Batteries**

Mr. Anthony T Pacileo M.S., Mr. Patrick Deegan, Dr. Hao Liu Ph.D.

Binghamton University, Binghamton, NY, USA

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4:05 - 4:20pm

**209 Fingerprinting the Water and Vacancy Sites in Superhydrous Hematite: Neutron Scattering and First Principles Studies**

Si Athena Chen Ph.D.[1], Bryan C. Chakoumakos Ph.D.[1], Prof. James D. Kubicki[2], Matthias D. Frontzek Ph.D.[1], Luke L. Daemen Ph.D.[1], Yuanpeng Zhang Ph.D.[1], Jeffrey E Post Ph.D.[3], Prof. Peter J. Heaney[4]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, USA. [2]University of Texas at El Paso, El Paso, Texas, USA. [3]Smithsonian Institution, Washington, D.C., USA. [4]Penn State University, State College, PA, USA

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4:20 - 4:35pm

**132 Hydrogen Storage with Aluminum Formate, ALF: Experimental, Computational, and Technoeconomic Studies**

Hayden Evans[1], Taner Yildirim[1], Peng Peng[2], Yongqiang Cheng[3], Zeyu Deng[4], Qiang Zhang[3], Dinesh Mullangi[4], Dan Zhao[4], Pieremanuele Canepa[5], Hanna Breunig[2], Anthony K Cheetham[6], Craig M Brown[1]

[1]NIST, Gaithersburg, MD, USA. [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA. [3]ORNL, Oak Ridge, TN, USA. [4]NUS, Singapore, Singapore, Singapore. [5]UH, Houston, TX, USA. [6]UCSB, Santa Barbara, CA, USA

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4:35 - 4:50pm

**81 Hide and Go Seek: Finding the Locations of Ca, Zn, and S ions within LTA Zeolite Modified for $H_2S$ Capture**

Adeyemi D Ojaide, Miles Bradford, Dr. Stacey J Smith Doctorate, Dr. Roger G Harrison Doctorate
Brigham Young University, Provo, Utah, USA

**Closing Celebration**
5:00 - 10:00pm Tuesday, 22nd July, 2025
Session Room: Offsite: City Cruises – Spirit of Chicago
Chairs Stacey Smith, Samantha Powell, Sarah Bowman, Christine Beavers
Reception Location
City Cruises – Spirit of Chicago
600 E Grand Ave, Chicago, IL 60611

Look for the “Spirit of Chicago” vessel docked at Navy Pier.

Schedule & Transportation

- 5:00 PM – Bus departs from the Westin Chicago Lombard
(70 Yorktown Shopping Center, Lombard, IL 60148)
final boarding is at 5:15 PM
If you miss the bus, you will need to arrange your own transportation to Navy Pier.
- 6:00 PM – Boarding begins at Navy Pier
- 6:30 PM – Boat launches and dinner begins
- 7:15 PM (approx.) – Closing remarks by ACA President Gerald Audette, awards presentations, and recognition of session chairs
- 9:30 PM – Boat returns to dock
- 10:00 PM – Return bus departs from Navy Pier back to the Westin
- 10:30 PM – Expected arrival at the Westin

Guests will enjoy a vibrant buffet dinner featuring entrées like citrus herb salmon, birria-style chicken, and spring garlic cream pasta—alongside fresh salads, seasonal sides, and a dessert station. Gluten-free, vegetarian, and some vegan options will be available.

Please wear your badge and bring any personal items you’ll need for the evening.

**HDRMX workshop: Data Rates and Metadata over the Next Decade**
9:00am - 5:00pm Wednesday, 23rd July, 2025
Session Room: Lilac A
Chairs Graeme Winter, Aaron Brewster
HDRMX (High Data Rate Macromolecular Crystallography) is a consortium of interested software developers, detector manufacturers, facility staff, beamline scientists, and users, who meet to discuss next-generation challenges in data acquisition, transfer, processing, storage, and provenance.

This full-day session will consist of short talks and longer discussion sections, featuring topics such as anticipated data rates, the necessary infrastructure for transfer and processing, plans for long-term storage, benefits and difficulties with lossy compression, metadata standards, and deficiencies, multi-modal experiments, an provenance for raw data, processing, and deposition.