



ACA: The Structural Science Society
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2021 Full Program w/ Abstract List

2021 ACA Meeting Committee:

N. Ando

C. Slebodnick

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A. Gardberg

Scientific sessions and workshops at the 2021 ACA Annual Meeting will highlight new developments in single-crystal and powder diffraction, scattering, cryo-EM, micro-electron diffraction, and advanced capabilities at national x-ray, neutron, and EM facilities.



It is a great honor to collaborate with the International Union of Crystallography (IUCr) each year to archive all of the abstracts submitted to the ACA Annual Meeting. Information on past meetings, including statistics, and the link to the archived abstracts can be found here: <https://www.amerystalassn.org/past-meetings>.

If there is an abstract that you would like to view please go to here: <https://www.amerystalassn.org/past-meetings>, click on the abstracts for the 2021 annual meeting and search the author or keyword. If you would like to search for the contact information for the author please sign into your ACA account and search by name (<https://acas.memberclicks.net/member-directory-mo#/>).

1.1.1 General Interest

7/31/2021

Session Chairs: Marc Giulanotti & Brandon Mercado

Sponsoring SIG: General Interest

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

Abstract Title: Electronic Structure-Property Relations of Photochromic MOFs from the Cambridge Crystallographic Structural Database

Presenting Author: Monu Joy, Clarkson University

Abstract Title: Single crystal diffraction beyond three dimensions: Dynamic structural responses of hydrogen-bonded materials using time filtering of event-based neutron TOF Laue diffraction

Presenting Author: Christopher Fancher, Material Science and Technology Division, Oak Ridge National Laboratory

Abstract Title: **Extending the structural space of quasicrystalline materials**
Presenting Author: **Kraig Wheeler, Dept of Chemistry, Whitworth University**

Abstract Title: **Pervasive approximate symmetry in organic [i]P[/i]1 structures**
Presenting Author: **Carolyn Brock, University of Kentucky**

Abstract Title: **Intramolecular Radical formation-induced chemical stability of novel ZW-MOFs**
Presenting Author: **Shefa Alomari, Clarkson university**

Abstract Title: **Metal-halide mediated radical generation and crystallization**
Presenting Author: **Mrittika Roy, University of California, Davis**

Abstract Title: **Historical notes on early neutron crystallography at the Oak Ridge Research Reactor**
Presenting Author: **Bryan Chakoumakos, Oak Ridge National Laboratory**

Abstract Title: **Photoreactivity and polymorphism of cinnamic acid revisited**
Presenting Author: **Dmitriy Soldatov, Chemistry, U of Guelph**

Abstract Title: **Visualization of the constellation of protons in the product-inhibited state of human manganese superoxide dismutase**
Presenting Author: **Jahaun Azadmanesh, Univ. Nebraska Medical Center**

Abstract Title: **The TELSAM Protein Polymer significantly Improves the Speed of Crystallization of target proteins**
Presenting Author: **sara soleimani**

Abstract Title: **Structural Science Awakens with a splash of water to the (inter)face**
Presenting Author: **Marcus Fischer, St. Jude Childrens Research Hospital**

1.1.1 General Interest 2

8/1/2021

Session Chairs: Victoria Drago & Brandon Mercado

Sponsoring SIG: General Interest

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

Abstract Title: **Using (3+1)D Space to Investigate a Modulated Superstructure Mystery**
Presenting Author: **Jeffrey Lovelace, Univ. of Nebraska Medical Center**

Abstract Title: **Peptidoglycan binding by a pocket on the accessory NTF2-domain of Pgp2 directs helical cell shape of Campylobacter jejuni**



Presenting Author: **Anson Chan, University of British Columbia**

Abstract Title: **Structural analysis of fibrillar polymorphs in AD (Alzheimer Disease) brain tissue and Pair distribution function of associated fibrils**

Presenting Author: **Prakash Nepal, Dept. of Bioengineering**

Abstract Title: **Solving protein structure using highly realistic diffraction photographs generated from MD trajectory of crystalline lysozyme**

Presenting Author: **Ning Liu, School of Life Sciences, Tsinghua University**

Abstract Title: **Structures of Synthetic Nanobodies in Complex with SARS-CoV-2 Spike or Receptor-Binding Domain Provide Insights for Developing Therapeutics and Vaccines**

Presenting Author: **Javeed Dhobi, National Institute of Health**

1.1.2 Mapping Free Energy Landscapes of Molecular Machines

7/31/2021

Chair(s): Kara Zielinski & Kevin Dalton

Sponsoring SIG: SAS

Co-Sponsoring SIGs: Young Scientist, Bio, Cryo-EM, Light Sources

X-ray scattering, cryo-EM, NMR, and diffraction experiments probing macromolecular structure away from energy minimum, i.e. by perturbing or exploring free energy landscape (t-jump, electric field, pressure, mixing, etc.).

Abstract Title: **Methods to Trap High-Temperature Conformations of Proteins using Fast Cooling**

Presenting Author: **Matthew McLeod, Cornell University**

Abstract Title: **Solution scattering and high-pressure biology**

Presenting Author: **Richard Gillilan, CHESS, Cornell Univ**

Abstract Title: **Investigating Photoreception, and Bio-catalysis using Time-resolved Serial Femtosecond Crystallography**

Presenting Author: **Suraj Pandey, University of Wisconsin - Milwaukee**

Abstract Title: **The important role of dynamics in the function and malfunction of molecular machines**

Presenting Author: **Lewis Kay**

Abstract Title: **Turning Up the Heat on Molecular Machines with Multi-Temperature and Temperature-Jump X-ray Scattering Experiments**

Presenting Author: **Michael Thompson, University of California, Merced**



1.1.3 Microcrystal Electron Diffraction

7/31/2021

Chair(s): Tamir Gonen & Xiaodong Zou

Sponsoring SIG: Small Molecule

Co-Sponsoring SIGs: Bio, Cryo EM, General Interest, Service

The field of microcrystal electron diffraction has rapidly progressed. Recent advances have placed microED at the forefront of structure determination. Several experimental protocols exist that describe the process of sequential sampling of diffraction patterns from nanometer-sized crystals while a sample is tilted in a transmission electron microscope. This session will be focused on advances in software/hardware and discussion of the results from microED experiments.

Abstract Title: MicroED application for GPCRs: structure of the human adenosine A2A receptor determined from a single nanocrystal in LCP

Presenting Author: **Anna Shiriaeva**

Abstract Title: Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures

Presenting Author: **Martin Seifrid**

Abstract Title: Structural analysis of polymorphs of small organic molecules by 3D ED/MicroED

Presenting Author: **Hongyi Xu, Department of Materials and Environmental Chemistry**

Abstract Title: Dynamical refinement: The way to improved fit, accurate structure models and absolute structure from 3D ED data.

Presenting Author: **Lukas Palatinus, Institute of Physics of the Czech Academy of Sciences**

Abstract Title: A simple pressure-assisted method for MicroED specimen preparation

Presenting Author: **Hongyi Xu, Department of Materials and Environmental Chemistry**

Abstract Title: Probing drug-protein interactions with MicroED

Presenting Author: **Lisa Clark, UCLA**

Abstract Title: MicroED with a direct electron detector

Presenting Author: **Johan Hattne, University of California, Los Angeles**

Abstract Title: DIALS data processing for MicroED

Presenting Author: **David Waterman, STFC**



1.1.4 Total Scattering: New Insights in Condensed Matter

7/31/2021

Chair(s): Matt Tucker & Peter Metz

Sponsoring SIG: M/N/P

While crystallography has traditionally dealt with the average, periodic arrangement of atoms in condensed matter, it has long been acknowledged that deviation from ideality is critically important to understanding macroscopic material phenomena. As atomic structure characterization tools have continued to mature, an increasing body of work has accumulated documenting locally perturbed atomic environments, even in materials of nominally high average symmetry. These studies are often complemented by spectroscopy and microscopy methods to confer a nuanced understanding of materials behavior and inform the materials science paradigm.

Beyond the classical examples of diffuse scattering, total scattering and the pair distribution function have been fruitfully applied to numerous contemporary materials science problems, including: ferroic materials, catalysts, strongly correlated electron systems, energy storage materials, as well as bulk/nanoscale variations on each theme.

New experimental techniques have also advanced local structure methodologies, particularly regarding advancements in grazing incidence X-ray PDF measurements of thin films, and advancements in the quantitative treatment of electron PDF data.

This symposium invites discussion of contemporary scientific developments enabled by local structure investigations of condensed matter.

Abstract Title: Materials on the nanoscale: Total scattering analysis for nanoparticle chemistry
Presenting Author: Kirsten Marie Jensen

Abstract Title: In situ grazing incidence total scattering: new in situ capabilities for pair distribution function analysis of thin films
Presenting Author: Ann-Christin Dippel, Deutsches Elektronen-Synchrotron DESY

Abstract Title: High Entropy Alloys local structure study by Reversed Monte Carlo method
Presenting Author: Wojciech Slawinski, University of Warsaw

Abstract Title: Probing the Local Atomic Structure of High-Entropy Oxides
Presenting Author: BO JIANG

Abstract Title: Tuning of disordered local structure in Prussian Blue analogues
Presenting Author: Arkadiy Simonov

Abstract Title: Elucidating Ionic Mobility in Multivalent Spinel Oxides
Presenting Author: Megan Murphy



Abstract Title: **Neutron PDF study of catalysts and battery materials: current status and future opportunities**

Presenting Author: **JUE LIU, Oak Ridge National Laboratory**

1.2.1 Instrumentation for Time-Resolved Experiments

8/1/2021

Chair(s): Robert Henning & Gisela Brändén

Sponsoring SIG: Light Sources

Time-resolved crystallography utilizes the bunch structure of the X-ray source to probe the structural dynamics over a range of time scales (femtoseconds to seconds). This requires highly specialized instrumentation that can take advantage of these unique sources, as well as purpose-build serial crystallography setups. This session will focus on the current & future instrumentation and experimental setups that are needed at synchrotrons and XFELs to do these types of experiments.

Abstract Title: **Protein synchronization methods and considerations: light activation and rapid mixing**

Presenting Author: **Diana Monteiro, Hauptman-Woodward Med. Res. Inst.**

Abstract Title: **Low background serial crystallography experiments**

Presenting Author: **Alke Meents, DESY**

Abstract Title: **Using the ALEX nylon mesh holder for time-resolved serial crystallography: successes and drawbacks.**

Presenting Author: **Darren Sherrell,**

Abstract Title: **What it Takes for a Successful Mix-and-Inject Serial Crystallography Experiment: From a Sample Preparation and Sample Delivery Perspective**

Presenting Author: **Kara Zielinski, Cornell University**

Abstract Title: **Solid-solid phase transition in adenine riboswitch crystals driven by large conformational changes induced by ligand**

Presenting Author: **Jason Stagno, Center for Structural Biology, Center for Cancer Research, National Cancer Institute**

Abstract Title: **Diffraction and scattering studies using high brightness Excillum MetalJet X-ray sources**

Presenting Author: **Anasuya Adibhatla, Excillum Inc**

Abstract Title: **Time-resolved x-ray scattering studies on the BioCARS beam line at the APS: the nuts and bolts of pushing the limits achievable at a synchrotron facility**

Presenting Author: **Philip Anfinrud, National Institutes of Health**



1.2.2 Materials for Sustainability and Energy

8/1/2021

Chair(s): Cheng Li

Sponsoring SIG: M/N/P

Crystallography lays the foundations for understanding the structure-property relationship of functional materials for energy and sustainability. Design and optimization of materials for energy conversion and storage technologies, such as batteries, fuel cell, thermoelectric and solar cell, relies upon insight of the crystal structure. This session will cover the latest development in the cross disciplinary fields of crystallography and materials science, so as to provide a discussion on the recent advance in the structural studies.

Abstract Title: Crystal Structure and Structure-Property Relationship of Halide Superionic Conductors as Solid Electrolyte for All-Solid-State Batteries

Presenting Author: **Hailong Chen**

Abstract Title: High entropy multication rock salt oxides for lithium ion batteries

Presenting Author: **Craig Bridges, Oak Ridge National Laboratory**

Abstract Title: Probing Structural Attributes for Li-Argyrodite as a Fast Ion Conductor using Neutron Powder Diffraction

Presenting Author: **Po-Hsiu Chien**

Abstract Title: Exploring aliovalent substitutions in the lithium halide superionic conductor $\text{Li}_{3-x}\text{In}_{1-x}\text{Zr}_x\text{Cl}_6$ ($0 \leq x \leq 0.5$)

Presenting Author: **Bianca Helm, University of Muenster**

Abstract Title: Salt Effects on Li-ion Exchange Kinetics and Activation Energies – Systematic In Situ Synchrotron Diffraction Studies

Presenting Author: **Christopher Bartel, University of California, Berkeley**

Abstract Title: Isoreticulation of Zwitterionic Metal-Organic Frameworks for Electrochromic Applications

Presenting Author: **John hadynski, Clarkson University**

Abstract Title: Understanding Selective Propane/Ethane Gas Adsorption using Neutron Diffraction

Presenting Author: **Benjamin Trump, NIST Center for Neutron Diffraction**



1.2.4 Redox Enzymes by Multiple Approaches

8/1/2021

Chair(s): Flora Meilleur & Jennifer Bridwell-Rabb

Sponsoring SIG: Biological Macromolecules

Redox enzymes are highly susceptible to radiation damage. Mitigation of X-ray induced perturbations of their metal centers or redox cofactors is key to structural investigation of their catalytic mechanisms. This session will discuss results from time resolved synchrotron, XFEL, and neutron crystallography as well as those from complementary techniques such as small angle scattering and computational calculations.

Abstract Title: **Direct detection of coupled proton and electron transfers in human manganese superoxide dismutase**

Presenting Author: **Gloria Borgstahl, The Eppley Inst For Cancer Res**

Abstract Title: **Structural basis of redox sensing by a cyanobacterial transcription regulator**

Presenting Author: **Bin Li**

Abstract Title: **Mutation to second sphere residue in peptidylglycine β -hydroxylating monooxygenase (PHM) reveals role of hydrogen-bonding network**

Presenting Author: **RENEE ARIAS, Oregon Health and Science University**

Abstract Title: **Redox modulation on chloroplast ATP synthase**

Presenting Author: **Po-Lin Chiu, Arizona State University**

Abstract Title: **MqsA antitoxin degradation is regulated by zinc occupancy and oxidation**

Presenting Author: **Benjamin Piraino, University of Rhode Island**

2.1.1 Evolving Enzymes

8/2/2021

Chair(s): Audrey Burnim & Ben Clifton

Sponsoring SIG: SAS

Co-Sponsoring SIG: Young Scientist

A session encompassing reconstructed (ancient) enzymes, directed evolution of synthetic functions, and structural biology with evolutionary context.

Abstract Title: **Ensemble epistasis: thermodynamic origins of non-additivity between mutations**

Presenting Author: **Michael Harms, University of Oregon**

Abstract Title: **On the contribution of substrate flexibility to define Methionine adenosyltransferase specificity**

Presenting Author: **Paola Laurino, Okinawa Inst. of Sci. & Tech. Graduate Univ.**



Abstract Title: **Meet the Family: Structural and Kinetic Comparisons of Representative PEPCKs**
Presenting Author: **Sarah Barwell, University of Waterloo**

Abstract Title: **Structural and dynamic basis for evolutionary bifurcations in enzyme families**
Presenting Author: **Colin Jackson, Research School of Chemistry**

Abstract Title: **Discovery and investigation of a naturally evolved fractal-like protein complex**
Presenting Author: **Franziska Sendker, Max Planck Institute for Terrestrial Microbiology**

Abstract Title: **Evolved and evolving allosteric regulation in the biosynthesis of aromatic amino acids**
Presenting Author: **Emily Parker, Victoria University of Wellington, Ferrier Research Institute**

2.1.3 Latest software developments in cryo-EM

8/2/2021

Chair(s): Charles Sindelar & Peijun Zhang

Sponsoring SIG: Cryo EM

This session will highlight recent developments in cryo-EM software for image processing and structure analysis, including topics such as: on-the-fly processing pipelines; higher resolution single-particle and tomographic structure determination; heterogeneity analysis; 3D reconstruction in situ; molecular modeling from density maps; and micro-electron diffraction for crystallographic structure determination.

Abstract Title: **Advances in heterogeneous reconstruction with cryoDRGN**
Presenting Author: **Ellen Zhong, MIT**

Abstract Title: **Singular value decomposition (SVD) of particle movements for motion analysis in cryoEM movies**
Presenting Author: **Raquel Bromberg, Ligo Analytics**

Abstract Title: **PySeg in Scipion: making easier template-free detection and classification of membrane-bound complexes in cryo-electron tomograms.**
Presenting Author: **Antonio Martinez-Sanchez, University of Oviedo**

Abstract Title: **Beam image-shift accelerated data acquisition for near-atomic resolution single-particle cryo-electron tomography**
Presenting Author: **Jonathan Bouvette, NIEHS**

Abstract Title: **Mapping atomic models back into cells - visual proteomics and in situ structure determination.**
Presenting Author: **Benjamin Himes**



Abstract Title: **Statistical estimation of spatially-resolved heterogeneity from cryo EM images**

Presenting Author: **Peter Doerschuk, Cornell University**

Abstract Title: **Interrogating macromolecular complex assembly by systematically analyzing the composition of highly heterogeneous structural ensembles**

Presenting Author: **Laurel Kinman, Massachusetts Institute of Technology**

Abstract Title: **Scipion for tomography: An expansion of Scipion software framework towards integration, reproducibility and validation in cryo-electron tomography.**

Presenting Author: **Federico de Isidro GÃ³mez, Spanish National Research Council**

Abstract Title: **Advances in modelling continuous heterogeneity from single particle cryo-EM data**

Presenting Author: **Ali Punjani, University of Toronto**

2.1.4 Magnetic Structure Determination: Advances and Applications

8/2/2021

Chair(s): Huibo Cao & William Ratcliff

Sponsoring SIG: M/N/P

Magnetic symmetry is key to understanding and designing many quantum and topological properties materials such as superconductors, quantum spin liquids, spin ices, topological insulators, chiral magnets, and skyrmions. The session will focus on various ideas on how to understand and design quantum and topological materials through magnetic and structural symmetries. We also welcome advanced magnetic and quantum characterization methods to enliven our discussions.

Abstract Title: **Revealing exotic magnetic states through machine learning assisted modeling of neutron diffuse scattering data**

Presenting Author: **David Tennant, Neutron Sciences Directorate, ORNL**

Abstract Title: **Reverse Monte Carlo refinement of single crystal diffuse neutron scattering and correlated magnetic disorder with program rmc-discord**

Presenting Author: **Zachary Morgan, Oak Ridge National Laboratory**

Abstract Title: **Magnetic vortices in a square lattice revealed by local magnetic susceptibilities and neutron diffuse scattering**

Presenting Author: **Erxi Feng, Oak Ridge National Laboratory**

Abstract Title: **Experimental Realization of Transverse Ising model on kagome and triangular lattice antiferromagnets**

Presenting Author: **Zhiling Dun**



Abstract Title: **Determine anisotropic g-tensor of rare-earth magnet using polarized neutron powder diffraction**

Presenting Author: **Xiaojian Bai**

Abstract Title: **Structural, magnetic ordering process and the magnetic excitations in spinel FeMn₂O₄**

Presenting Author: **Wei Tian, ORNL**

Abstract Title: **Centers of Spatial and Time Inversion Symmetry in Magnetoelectric Crystalline Materials**

Presenting Author: **Stephanie Gnewuch, University of Maryland, College Park**

Abstract Title: **MnBi₂Te₄.nBi₂Te₃: a happy marriage of magnetism and topology**

Presenting Author: **Ni Ni, university of california, los angeles**

Abstract Title: **La₂O₃-type structure magnetic topological candidates**

Presenting Author: **Madalynn Marshall, Rutgers University**

Abstract Title: **Magnetic properties in new half-Heusler-type compound**

Presenting Author: **Xin Gui, Princeton University**

2.1.5 Rosalind Franklin: 101st Anniversary

8/2/2021

Chair(s): Elspeth Garman & Joseph Orgel

Sponsoring SIG: BioMac

Co-Sponsoring SIG: Fiber

It is 101 years since the birth of Rosalind Franklin, famous for her part in defining the structure of DNA. However, this achievement constituted only a small part of her scientific output in a career that was sadly cut short due to her untimely death at the age of 37.

In this session, we will explore her foundational contributions to X-ray diffraction methods and crystallographic approaches. This is in addition to her role in advancing our understanding of the chemistry of coal, of the structure of DNA and of the three-dimensional arrangements of viruses.

Abstract Title: **Rosalind Franklin's pivotal research on coal, DNA and viruses.**

Presenting Author: **Elspeth Garman, Biochemistry, Oxford Univ**

Abstract Title: **First observation of aromatic bond density: a forgotten paper by Rosalind E. Franklin**

Presenting Author: **Alexander Nazarenko, Chemistry Dept, SUNY Buffalo State**

Abstract Title: **Rosalind Franklin and the Structure of Graphitic Carbons**

Presenting Author: **Margaret Schott, Northwestern University**



Abstract Title: **Rosalind Franklin and DNA**

Presenting Author: **Brian Sutton**

Abstract Title: **Rosalind Franklin, Still Guiding the Development of Carbon Based Materials**

Presenting Author: **Thomas Fitzgibbons, Analytical Sciences, The DOW Chemical Company**

Abstract Title: **Rosalind Franklin and her legacy in structural biology; the TMV chapter**

Presenting Author: **Gerald Stubbs, Vanderbilt University**

2.1.6 Economics of Crystallography

8/4/2021

Chair(s): Lee Daniels & Amy Sarjeant

Sponsoring SIG: Service

Scientists cannot escape the restraint imposed by the cost of their research. This half-day session examines the past, current and future states of funding and profit in the world of structural science. The organizers encourage input from academia, industry, government and non-profit agencies in order to clarify the present and future of our science. Topics may include: How does funding drive the need and availability of crystallographic results? Why support crystallography? Funding a service lab, and justifying the cost. How does a contract research lab make the service economically feasible? Pharmaceuticals: What are the costs of exploring salts, co-crystals and polymorphs? What are the risks of NOT producing solid crystalline products?

Abstract Title: **Role of Crystallography in Pharmaceutical Solid Form Development**

Presenting Author: **Rajni Bhardwaj, Abbvie**

Abstract Title: **Largest Problem: Getting a crystal and what is it worth to the researcher to have the 3D crystalline structure? Academic and Industrial Aspects.**

Presenting Author: **Richard Staples, Dept of Chemistry, Michigan State Univ**

Abstract Title: **Running a non-profit shared core facility**

Presenting Author: **Chris Malliakas, Northwestern University**

Abstract Title: **X-ray Crystallography at a Small Canadian University – A Personal Perspective**

Presenting Author: **Melanie Pilkington, Brock University**

Abstract Title: **Diffraction in the Context of the National Science Foundation (NSF)**

Presenting Author: **Carlos Murillo, NSF**



2.2.1 AI, Machine Learning, and Other Data Science Techniques Applied to Structure Determination

8/3/2021

Chair(s): Thomas Proffen

Sponsoring SIG: M/N/P

Advances in machine learning (ML) and artificial intelligence (AI) are already having a revolutionizing impact in many areas such as image, speech recognition or advancing self-driving cars. These techniques are starting to have an impact in materials science and beyond. This session will provide an overview of the impact of AI, ML and related methods are having on the field of crystallography now and in the future.

Abstract Title: Interpretable Machine Learning of Voluminous Scattering data

Presenting Author: Eun-ah Kim, Cornell University

Abstract Title: Sample Centering Using Google Cloud Platform's AutoML Vision.

Presenting Author: Scott Classen, Advanced Light Source

Abstract Title: Beamline Science â€” The Video Game: How Reinforcement Learning and Artificial Intelligence are Changing Operations at Large-Scale User Facilities

Presenting Author: Daniel Olds, Brookhaven National Laboratory

Abstract Title: CryoDiscovery (TM): A Machine Learning Platform for Automated Cryo-electron Microscopy 2D Class Selection

Presenting Author: Narasimha Kumar, Health Technology Innovations

Abstract Title: Emap2sec+: Detecting Protein and DNA/RNA Structures in Cryo-EM Maps of Intermediate Resolution Using Deep Learning

Presenting Author: Xiao Wang

2.2.2 Computing & Data Management

8/3/2021

Chair(s): Herbert J Bernstein & Dale Kreitler

Sponsoring SIG: Best Practices

Co-Sponsoring SIG: Bio

This is a half day session on Computing and Data Management (CDM) with talks relating to useful methods in computing and data management (not just nice results) as a companion to another half day session on Meeting the Challenges of Raw Data Management (MCRD).

CDM will focus on methods now coming to the fore in solving crystallographic structures, including advances in improving and speeding up crystallographic pipelines, advances in using models and AI in starting and managing the solution process, advances in disaggregating data from multiple conformations and states, advances in integrating results from multimodal experiments across multiple scales, etc.



Abstract Title: **Discrete conformations of an enzyme are discernible via hierarchical clustering of X-ray diffraction intensities derived from multiple crystals**

Presenting Author: **Dale Kreitler, National Synchrotron Light Source II**

Abstract Title: **Approximate Lattice Similarity**

Presenting Author: **Larry Andrews, Ronin Institute**

Abstract Title: **Scaling up: processing XFEL data at kilohertz speeds using cctbx.xfel**

Presenting Author: **Aaron Brewster, Lawrence Berkeley National Lab**

Abstract Title: **Literate programming with CCTBX and PyMOL in Jupyter notebooks**

Presenting Author: **Blaine Mooers, University of Oklahoma Health Sciences Center**

Abstract Title: **The Life and Times of the PDB Format - Looking Towards the Future with mmCIF**

Presenting Author: **Gregg Crichlow**

2.2.3 Economics of Crystallography

7/31/2021

Chair(s): Lee Daniels & Amy Sarjeant

Sponsoring SIG: Service

Scientists cannot escape the restraint imposed by the cost of their research. This half-day session examines the past, current and future states of funding and profit in the world of structural science. The organizers encourage input from academia, industry, government and non-profit agencies in order to clarify the present and future of our science. Topics may include: How does funding drive the need and availability of crystallographic results? Why support crystallography? Funding a service lab, and justifying the cost. How does a contract research lab make the service economically feasible? Pharmaceuticals: What are the costs of exploring salts, co-crystals and polymorphs? What are the risks of NOT producing solid crystalline products?

Abstract Title: **Building a crystallographic instrument company - planning and serendipity**

Presenting Author: **Susan Byram, Crystallographic Systems, Bruker AXS Inc**

Abstract Title: **From lab to synchrotron and back: could better, faster and newer also be more economical?**

Presenting Author: **Dubravka Sisak Jung, Dectris Ltd**

Abstract Title: **The Journey of Macromolecular Crystallography in Pharmaceutical Discovery Research at Abbvie and BMS.**

Presenting Author: **Jodi Muckelbauer, Molecular Structure & Design, Bristol-Myers Squibb**

Abstract Title: **The Changing Economics of an Academic Structural Biology Core Facility**

Presenting Author: **Diana Tomchick, UT Southwestern Medical Center**



Abstract Title: **Pushing the Boundaries in Crystallization Screening: Making Automated, User-accessible Crystallization Work**

Presenting Author: **Sarah Bowman, HWI**

2.2.4 Membrane protein structure in membrane and membrane-mimic environments

8/3/2021

Chair(s): Kushol Gupta & Venky Pingali

Sponsoring SIG: SAS

Membrane proteins play a critical role in numerous cellular-related functions such as cell-cell signaling, molecular transport through membranes, and the anchoring of the cytoskeleton. Therefore, elucidation of membrane protein structure is essential to the understanding of their function. However, membrane proteins are not stable in aqueous buffer solutions without a stabilizing vehicle such as lipid membranes, surfactant micelles, bicelles, and even non-natural polymers. This session will present research catering to the various membrane and membrane-mimic environments employed for the study of membrane proteins, as well as the methodologies developed to expand the frontiers of the study of membrane protein structure and function.

Abstract Title: **Small angle x-ray scattering of the intrinsic tenase complex bound to lipid nanodisc provides insight into intermolecular contacts between factors VIIIa/IXa**

Presenting Author: **Kenneth Childers, Western Washington University**

Abstract Title: **Bicontinuous microemulsion (B μ E) as a membrane-mimic to stabilize and enable structural studies of membrane proteins**

Presenting Author: **Sai Venkatesh Pingali, Oak Ridge National Laboratory**

Abstract Title: **The Dynamic Interplay between Cell Membranes and Membrane Proteins**

Presenting Author: **Rana Ashkar, Virginia Tech**

Abstract Title: **SMALL-ANGLE NEUTRON SCATTERING FOR INTEGRATIVE STRUCTURAL MODELING OF MEMBRANE PROTEINS IN CIRCULARIZED NANODISCS**

Presenting Author: **Kaitlyn Ledwitch, Vanderbilt University**

Abstract Title: **Neutron reflectometry of peripheral membrane proteins on biomimetic membranes: capabilities and examples**

Presenting Author: **David Hoogerheide, National Institute of Standards and Technology**



2.2.5 What can & can't we see reliably at resolution X?

8/3/2021

Chair(s): Jane Richardson & Nigel Moriarty

Sponsoring SIG: Cryo EM

Co-Sponsoring SIG: Bio

Most structural biologists are familiar with what features can be seen in x-ray crystal structures of proteins in the commonest range around 2Å resolution and have sometimes been frustrated by what we cannot see at all clearly at 3Å or worse. This session will emphasize both new studies about similarities and differences for cryo-EM (or even neutron diffraction), and also new methods that can now let us do better than expected in some cases.

Abstract Title: **Introduction to 'What can and can't we see'**

Presenting Author: **Jane Richardson, Duke University**

Abstract Title: **Interpretation of RNA cryo-EM maps of various resolutions**

Presenting Author: **Rhiju Das, Stanford University**

Abstract Title: **Adapting to varying resolutions in ISOLDE**

Presenting Author: **Tristan Croll, University of Cambridge**

Abstract Title: **Outcomes from EMDDataResource Model Challenges**

Presenting Author: **Catherine Lawson, Institute for Quantitative Biomedicine, Rutgers Univ**

Abstract Title: **What are the current limits on determination of protonation state using neutron MX?**

Presenting Author: **Dorothee Liebschner, Lawrence Berkeley National Laboratory**

2.3.1 Open exchanges in crystallographic education

8/1/2021

Chair(s): Andrew Torelli & Kraig Wheeler

Sponsoring SIG: General Interest

Crystallographic education is vital to every aspect of our profession from the training of current and next generation scientists to the potential for shaping public perceptions. This session offers an informal platform for speakers to communicate their approaches and techniques that promote the learning process of crystallography. The short format of this session (10 minute talks) will encourage speakers and attendees to freely share ideas on focused topics that range from innovative hands-on exercises, virtual resources, and novel must-have classroom modules.

Abstract Title: **XrayView: A teaching aid for X-ray crystallography**

Presenting Author: **George N. Phillips, Jr., Rice University**



Abstract Title: **Engaging diverse students with Crystallography Research**
Presenting Author: **Oluwatoyin Asojo, Hampton University**

Abstract Title: **Integrating Chemical Crystallography into Undergraduate Laboratories: A Remotely Conducted Discovery Based Molecular Structure Determination Lab Module**
Presenting Author: **Joe Tanski, Vassar College**

Abstract Title: **Crystallographic Literacy at American Crystallographic Association**
Presenting Author: **Allen Oliver, Dept of Chemistry & Biochemistry, Univ of Notre Dame**

Abstract Title: **Integrating Crystallography in Undergraduate Lab Experiences**
Presenting Author: **Charlotte Stern, Northwestern University**

Abstract Title: **Adventures in structural chemistry education: techniques for teaching crystallography virtually**
Presenting Author: **Yinka Olatunji-Ojo, The Cambridge Crystallographic Data Centre**

Abstract Title: **A blended learning approach for a crystallography-based undergraduate practical [under COVID-19 restrictions]**
Presenting Author: **Peter Horton, University of Southampton**

Abstract Title: **Protein Crystallography & PUIs**
Presenting Author: **Krystle McLaughlin, Vassar College**

Abstract Title: **A Video Demonstration of a Single Crystal X-Ray Determination of Sugar**
Presenting Author: **Alain Beuparlant, East Tennessee State University**

Abstract Title: **The Use of Blender and SketchFab to Create and Share Teaching Tools for Crystallography**
Presenting Author: **Michael Aristov, Chemistry, UW Madison**

3.1.1 Advances in Detector Technology

8/4/2021

Chair(s): Joseph Ferrara & Christopher Russo

Sponsoring SIG: Cryo EM

Co-Sponsoring SIG: Best Practices

The detection of X-rays, neutrons, and electrons for diffraction and imaging techniques has changed dramatically over the last 20 years. This half-day session will explore the most recent advances in detector technology as they apply to imaging and diffraction techniques.

Abstract Title: **Challenging the limits of detection technology**
Presenting Author: **Marcus Mueller, DECTRIS Ltd.**



Abstract Title: **A large area photon counting X-ray detector with indirect conversion**
Presenting Author: **Roger Durst, Bruker AXS GmbH**

Abstract Title: **Development of a Large Area Fast Readout HPC Detector**
Presenting Author: **Yasukazu Nakaye, Rigaku Corporation**

Abstract Title: **New developments in Time-of-Flight Neutron Detectors at Oak Ridge National Lab**
Presenting Author: **Richard Riedel, Oak Ridge National Lab**

Abstract Title: **Charge-integrating hybrid pixel array detectors for x-ray science and electron microscopy**
Presenting Author: **Kate Shanks, Cornell High Energy Synchrotron Source**

Abstract Title: **Hybrid-Pixel Detection and Software Automation Streamlining Electron Diffraction Experiments**
Presenting Author: **Anahita Pakzad**

Abstract Title: **Falcon 4 performance validation by single event analysis**
Presenting Author: **Jeffrey Lengyel**

3.1.2 Complementarity among structural methods

8/4/2021

Chair(s): Carlos Escalante

Sponsoring SIG: Biological Macromolecules

Co-Sponsoring SIGs: General Interest, M/N/P, Small Molecule

Recent advances in many structural biology techniques are allowing the study of more complex structures that were previously intractable. Moreover, the complementary of information provided by different techniques provides a better justification of the structure as it may integrate the static and dynamic information of a particular system. The aim of this session to present recent examples where a combination of techniques such as X-ray crystallography, SAXS, NMR spectroscopy, Cryo-Electron Microscopy among others, has been used successfully to tackle complex and dynamic structures of biological importance.

Abstract Title: **MAINMAST: De Novo Protein Structure Modeling for cryo-EM Maps Assisted by Structure Feature Detection by Deep Learning**
Presenting Author: **Genki Terashi, Department of Biological Sciences, Purdue University**

Abstract Title: **Structural insight into dual function of Neisserial lactoferrin binding protein B**
Presenting Author: **Ravi Yadav, Purdue University**

Abstract Title: **Structural Insights into Outer Membrane Protein Biogenesis in Pathogenic Neisseria**



Presenting Author: **Evan Billings, Purdue University**

Abstract Title: **Toward elucidating the mechanism of lytic polysaccharide monooxygenases: Chemical insights from X-ray and neutron crystallography**

Presenting Author: **Gabriela Schroder**

Abstract Title: **Understanding conformational changes in MCM-family helicases through experimental structures and SVD-based metadata analysis**

Presenting Author: **Heewhan Shin**

3.1.5 What I Learned from My First Structures

8/4/2021

Chair(s): Silvana Urcia-Romero & Larry Falvello

Sponsoring SIG: Service

Co-Sponsoring SIG: Small Molecule

This session aims to trace the development of the methodologies used in structure analysis in terms of the techniques applied by different generations of crystallographers. This will provide a developmental context for the technology, techniques and practices used today. The skills learned by each one of us for our first structure analyses serve as a time stamp for the starting point of our work in crystallography. The continual improvement of these techniques is chronicled by the changing practices in X-ray structure analysis. A high level of technical involvement by the user decades ago, and the accompanying imperative for the user to perfect all details of the results to the extent possible, have receded with the evolution of automated rapid-throughput analysis accompanied by quality control in the form of computerized validation. At the same time, analysis that were considered unfeasible years ago, involving twinning, modulation, ab-initio powder diffraction analysis and others, can be undertaken with relative ease today. That evolution of techniques and tools has also transformed the user's educational point of view, changing the emphasis in training from technical acuity with instrumentation, software, and fundamental crystallography itself, to a stronger focus on the results and their implications in a broader scientific context. Presentations will outline what has been achieved so far by past and present generations, including reference to fundamental details that are no longer considered explicitly. Submissions are welcome from all experience levels.

Abstract Title: **Lessons in Translational Non-Crystallographic Symmetry: Solving the Crystal Structure of a Putative Protease from *Gemella haemolyans***

Presenting Author: **Norman Tran**

Abstract Title: **Cannabidiol: A natural product structure in the mid-1970s. Weissenberg photos, four-circle diffractometry, direct methods, and more**

Presenting Author: **Larry Falvello, Dept of Inorganic Chemistry, Univ of Zaragoza**

Abstract Title: **Anecdotal Lessons from the 1990's**

Presenting Author: **Carla Slebodnick, Dept of Chemistry, Virginia Tech**



Abstract Title: **First structures as undergraduate and graduate student**
Presenting Author: **Raúl Castañeda, New Mexico Highlands University**

Abstract Title: **Solving a structure as a goal vs. solving a structure as a tool. Learning crystallography along evolving times.**
Presenting Author: **Leopoldo Suescun, Universidad de la República, Facultad de Química, Uruguay**

Abstract Title: **Darkrooms, paper tape, punch cards and grease pencils: Doing crystallography at Caltech in the early 1970s**
Presenting Author: **Frank Fronczek, Dept of Chemistry, Louisiana State Univ**

Abstract Title: **Jumping in the deep end: 1970s structural challenges and their impact for a career in crystallography teaching and research**
Presenting Author: **William Clegg, Chemistry, School of Natural and Environmental Sciences, Newcastle Univ**

Abstract Title: **Four lessons from my very early days in crystallography: The lasting impact of a few selected first structures on my path in science.**
Presenting Author: **Bruce Foxman, Chemistry MS015, Brandeis Univ**

3.2.3 Evolution and Impact of Targeted Protein Degradation in Industry

8/5/2021

Chair(s): Matt Clifton & Joe Patel

Sponsoring SIG: Industrial

Targeted protein degradation denotes the ability of a small molecule to catalyze the selective breakdown of a protein of interest via the ubiquitin-proteasome system (UPS). The ability to modulate protein levels offer a novel alternative paradigm to classical inhibitors and has been a major focus for both industrial and academic groups around the world. Structural characterization of these small molecule induced, non-cognate ternary complexes between the E3 ligase and protein of interest has presented unique challenges to advancing structure-based drug design efforts. This session will be dedicated to highlighting the significant structural advances that have been made in interrogating these induced complexes, insights into the structure-activity relationships of the small molecules, and the plasticity of the ligases to selectivity recognize disease relevant targets.

Abstract Title: **Structure-Function Studies on Cereblon and the Implications for Novel Molecular Glue Discovery**
Presenting Author: **Philip Chamberlain, Neomorph, Inc.**

Abstract Title: **Structure based design of degraders.**
Presenting Author: **Radoslaw Nowak, Dana-Farber Cancer Institute**



Abstract Title: **Snapshots and ensembles of BTK and cIAP1 protein degrader ternary complexes**

Presenting Author: **Matthew Calabrese**

Abstract Title: **Discovery and structural characterization of a VHL-mediated molecular glue degrader targeting cysteine dioxygenase**

Presenting Author: **Xiaolei Ma, Novartis Institutes for BioMedical Research**

Abstract Title: **Finding a way out of the Labyrinth: Degrader induced ternary complex modelling**

Presenting Author: **Jenifer Winters, C4 Therapeutics**

Abstract Title: **Ternary PROTAC structures necessary and sufficient?**

Presenting Author: **Chun-wa Chung, GlaxoSmithKline R&D**

3.2.4 Getting the first crystal

8/5/2021

Chair(s): Sarah Bowman & Janet Newman

Sponsoring SIG: Biological Macromolecules

Co-Sponsoring SIGs: Canadian, Young Scientist

Crystallography needs high-quality, well-diffracting crystals – this is a rate limiting step in crystal based structure determination. In this session we will discuss screening strategies, developing new crystallization screens, seeding, modulating a protein construct to make it ‘more crystallizable’, strategies for membrane proteins, strategies for ‘seeing’ crystals, etc. Do you have a good ‘getting the first crystal’ story about a system you are working on? Do you have a strategy that works almost all of the time? We welcome submission of abstracts on these topics.

Abstract Title: **The ideal crystal for structural biology**

Presenting Author: **Edward Snell, Hauptman-Woodward Medical Research Institute/BioXFEL**

Abstract Title: **Crystallization Conditions in the Protein Data Bank**

Presenting Author: **Deborah Harrus, EMBL-EBI**

Abstract Title: **Data and Diversity Driven Development of a Shotgun Crystallisation Screen using the Protein Data Bank**

Presenting Author: **Gabriel Abrahams**

Abstract Title: **POLO: A web interface for the rapid identification of crystals**

Presenting Author: **Charles Lesburg, Merck & Co., Inc.**

Abstract Title: **Fusion to the TELSAM Protein Polymer Dramatically Improves the Speed of Target Protein Crystallization by Stabilizing Weak Crystal Contacts**

Presenting Author: **James Moody**



Abstract Title: **A comprehensive strategy for efficient generation of well-diffracting crystals**
Presenting Author: **Miki Senda, High Energy Accelerator Research Organization (KEK)**

Abstract Title: **Plug-and-play polymer microfluidic chips for hydrated, room-temperature fixed-target serial crystallography.**

Presenting Author: **Deepshika Gilbile, University of California Davis**

3.2.5 Quantum Materials: Magnetism, Correlation, and Topology in Condensed Matter

8/5/2021

Chair(s): Jared Allred & Benjamin Frandsen

Sponsoring SIG: M/N/P

In quantum materials, non-trivial quantum mechanical states give rise to unusual macroscopic properties. Quantum materials stretch our understanding of the fundamental physics of materials and, in many cases, hold tremendous promise for eventual technological application. This class of materials includes topological materials, spin liquids, and other magnetic and/or correlated electron systems. The intriguing emergent phenomena observed in such systems can be heavily dependent on the physical structure, where even subtle details can have significant impact. This session will emphasize how crystallographic tools have been or can be used to uncover the structure-property relationship in quantum materials.

Abstract Title: **How the Coupled Spin, Orbital and Lattice Degrees of Freedom Can Cause Happiness or Distress in Asymmetric Magnetic Exchange Interaction, and Why It Matters for Microelectronic Applications**

Presenting Author: **Thao Tran, Clemson University**

Abstract Title: **Nematicity in a local-moment iron chalcogenide**

Presenting Author: **Yu Song, University of California, Berkeley**

Abstract Title: **Understanding Quantum Materials Under Extreme Sample Environments**

Presenting Author: **Sara Haravifard, Duke University**

Abstract Title: **Switchable Rashba anisotropy in a layered hybrid organic-inorganic perovskite via hybrid improper ferroelectricity**

Presenting Author: **Branton Campbell, Brigham Young University**

Abstract Title: **Evolving charge density wave and band structure control in topological semimetals $\text{LnSb}_x\text{Te}_{2-x}$ ($\text{Ln} = \text{Ce}, \text{Nd}, \text{Gd}$)**

Presenting Author: **Tyger Salters, Princeton University**



Abstract Title: **Crystallography of Lithiated and Delithiated Transition Metal Phosphates and Thiophosphates**

Presenting Author: **Timothy Diethrich, University of Maryland, College Park**

Abstract Title: **Tuning the magnetism and band topology through antisite defects in Sb doped MnBi₄Te₇**

Presenting Author: **Chaowei Hu, University of California, Los Angeles**

Abstract Title: **Broken-helix antiferromagnetic order protecting a crystalline axion insulator phase and exotic surface states in EuIn₂As₂.**

Presenting Author: **Simon Riberolles, Ames Laboratory**

Abstract Title: **Novel Iridates Single Crystals Grown under High Pressure**

Presenting Author: **Weiwei Xie, Rutgers University - Piscataway**

Abstract Title: **Scattering Signatures of Bond-Dependent Magnetic Interactions**

Presenting Author: **Joseph Paddison, Oak Ridge National Laboratory**

4.1.1 BioWAXS: experiment and interpretation

8/5/2021

Chair(s): Steve Meisburger & Jochen Hub

Sponsoring SIG: SAS

The molecules of life are in constant motion. To gain insight into dynamics on the atomic scale, it is increasingly common to apply wide-angle X-ray scattering (WAXS) to biomolecular solutions or condensed phases, especially in conjunction with time-resolved experiments. The WAXS signal is uniquely sensitive to dynamic structural fluctuations and hydration effects, both of which are key to a mechanistic understanding of function. However, the challenge of interpreting the WAXS signal has traditionally limited its biological applications. In recent years, the challenge has been addressed through a combination of new experimental techniques (such as temperature-jump and X-FEL) and sophisticated computational approaches (such as ensemble fitting, physics-based modeling, and machine learning). In this session, we aim to advance the field by highlighting recent experimental results and new methods for interpretation.

Abstract Title: **Revealing structural dynamics of proteins with time-resolved x-ray liquidography**

Presenting Author: **Hyocheol Ihee, Dept of Chemistry, KAIST, & Inst for Basic Science**

Abstract Title: **Probing photoinduced protein function by time resolved X-ray scattering**

Presenting Author: **Giorgio Schiro, IBS - CNRS**

Abstract Title: **Instrumentation and applications of simultaneous SAXS/WAXS at the LiX beamline**

Presenting Author: **Lin Yang, Brookhaven National Laboratory**



Abstract Title: **Classification of tissue variations in X-ray scanning microdiffraction from thin sections of human brain**

Presenting Author: **Abdullah Al Bashit, Northeastern University**

Abstract Title: **Decoding hidden structural information in solution wide-angle X-ray scattering (WAXS): from ensemble modeling to machine learning**

Presenting Author: **Yen-Lin Chen, Cornell University**

Abstract Title: **Visualization of biomolecular structures by WAXS and MD**

Presenting Author: **Weiwei He, New York University**

Abstract Title: **Probing structural dynamics of biomolecules in solution at high resolution via time-resolved small- and wide-angle x-ray scattering**

Presenting Author: **Philip Anfinrud, National Institutes of Health**

4.1.2 Cool Structures

8/3/2021

Chair(s): Nichole Valdez & Steven Kelly

Sponsoring SIG: Small Molecule

This session aims to both highlight interesting structures of small molecules (<100 atoms permolecule) and bring to the foreground the science enabled by small-molecule structure analysis. Speakers will be selected from contributed abstracts. Submissions from students are encouraged.

Abstract Title: **Understanding Intermetallic Intergrowths and Reactivity: Chemical Pressure-Driven Epitaxy Between Domain Interfaces**

Presenting Author: **Kyana Sanders, University of Wisconsin, Madison**

Abstract Title: **Fully fluorinated Pd(F6acac) complexes: polymorphism and fluorine-fluorine interactions.**

Presenting Author: **Veronica Carta, Indiana University**

Abstract Title: **Small Molecule Microcrystal Electron Diffraction (MicroED) for the Pharmaceutical Industry Lessons Learned from Examining Over Fifty Samples**

Presenting Author: **Jessica Bruhn, Nanomaging Services**

Abstract Title: **The First X-ray Crystal Structures of 5,5,10,10-Tetrahalotricyclo[7.1.0.0^{sup}4,6^{/sup}]]decanes**

Presenting Author: **Kent Clinger**

Abstract Title: **The Many Moods of the 3-Aminopyridinium Chlorocuprate(II) System**

Presenting Author: **Marcus Bond, Dept of Chemistry and Physics, Southeast Missouri State University**



Abstract Title: **Variable Temperature Polymorphism of 2-benzoyl-N,N-diethylbenzamide**

Presenting Author: **Lygia Silva de Moraes, University Libre de Bruxelles**

Abstract Title: **Water Soluble Picolamidine Metal Complexes**

Presenting Author: **Raúl Castañeda, New Mexico Highlands University**

4.1.4 Large-Scale Facility Upgrades

8/2/2021

Chair(s):

Ana Gonzalez, John Chrzas & Bryan Chakoumakos

Sponsoring SIG: Light Sources

Large scale light and neutron sources must undergo upgrades in order to satisfy users requirements and to remain competitive in response to the development of new state of the art sources. This session will report on some of the recently achieved and planned upgrades, the challenges to overcome and the new experimental possibilities that these projects enable in the field of diffraction based applications.

Abstract Title: **High energy upgrade of the Linac Coherent Light Source**

Presenting Author: **Andrew Aquila, SLAC National Accelerator Laboratory**

Abstract Title: **Neutron Diffractometer Concept(s) for the Second Target Station at the Spallation Neutron Source***

Presenting Author: **Yaohua Liu, Oak Ridge National Laboratory**

Abstract Title: **Conceptual Design of a Small- and Wide-angle Neutron Scattering Diffractometer/Spectrometer for the Second Target Station of the SNS: Centaur**

Presenting Author: **SHUO Qian, Oak Ridge National Laboratory**

Abstract Title: **The APS upgrade offering new opportunities for materials science**

Presenting Author: **Uta Ruett, Argonne National Laboratory**

Abstract Title: **NSFs ChemMatCARS - Advanced Crystallography Program A Dedicate Advanced Small Molecule Crystallography Beamline**

Presenting Author: **Yu-Sheng Chen, University of Chicago**

Abstract Title: **SERCAT-BCSB Collaboration During SER-CAT/APS Upgrade**

Presenting Author: **Bi-Cheng Wang, University of Georgia**

Abstract Title: **The ID29 upgrade project: a new serial crystallography beamline for time resolved studies at ESRF-EBS**

Presenting Author: **Daniele de Sanctis, ESRF**



Abstract Title: **Warmer, deeper, wider: New developments at MacCHESS**
Presenting Author: **Doletha Szebenyi, MacCHESS, Cornell Univ**

4.1.5 Structural Biology of Infectious Diseases

8/3/2021

Chair(s):

George Lountos & Jason Mclellan

Sponsoring SIG: Biological Macromolecules

Co-Sponsoring SIGs: Cryo-EM and Industrial

This session will focus on the structural basis of host–pathogen interactions and the application of structural biology to combat infectious diseases. Possible topics include, but are not limited to, structural studies on viral, bacterial, and fungal proteins and their mechanisms of action or interactions with host cell molecules, receptors, and antibodies. Structure-based vaccine and antibody development is also of interest.

Abstract Title: **Recognition of the Plasmodium spp. circumsporozoite protein by malaria inhibitory antibodies**

Presenting Author: **Iga Kucharska, The Peter Gilgan Centre for Research and Learning, Hospital for Sick Children**

Abstract Title: **Structurally investigating a niche pathway for chemical reversal of proline hydroxylation in the pathogen C. difficile**

Presenting Author: **Lindsey Backman, Massachusetts Institute of Technology**

Abstract Title: **Structures of Usutu SAAR-1776 virus: a comparison with known structures of mature flaviviruses**

Presenting Author: **Baldeep Khare, Purdue University**

Abstract Title: **Constraining Evolution â€˜ Avoiding Drug Resistance: Lessons from Viruses**

Presenting Author: **Celia Schiffer, University of Massachusetts Medical School**

Abstract Title: **Deploying high-throughput protein crystallography-based drug discovery platforms to establish a structure-based drug discovery system for SARS-CoV-2 proteins**

Presenting Author: **Debanu Das, Accelero Biostructures**

Abstract Title: **Direct visualization of SARS-CoV-2 main protease electrostatics using neutron crystallography**

Presenting Author: **Stephanie Galanie, Oak Ridge National Lab**

Abstract Title: **SARS-CoV-2 ferritin nanoparticle vaccines elicit broad SARS coronavirus immunogenicity**

Presenting Author: **michael joyce, Henry M. Jackson Foundation / Walter Reed Army Institute of Research**



4.2.2 Meeting the Challenges of Raw Data Deposition

8/4/2021

Chair(s): John Rose & Wladek Minor

Sponsoring SIG: Best Practices

Co-Sponsoring SIG: Bio

The ability reproduce experimental results (the basis of a publication or other scholarly work) strongly relies on the availability of primary experimental data. The Structural Biology community recognizes this and has encouraged the sharing of research data since its birth.

Today, the importance of archiving the raw data (the images and their associated metadata) leading to a structure has come to the forefront as reflected by the work of the IUCr and the ACA in this area. In addition, funding agencies are particularly interested in the reproducibility of the work they fund.

The speakers in the session will describe the crucial role that diffraction data may play in providing raw data needed for improving data reduction software leading to better structures, the re-determination of suboptimal macromolecular structures to improve structure quality and providing a reproducible platform for extending these analyses by future investigators.

Abstract Title: Integrated Resource for Reproducibility in Molecular Crystallography: experiences of the first five years

Presenting Author: Marek Grabowski, University of Virginia

Abstract Title: Ice in Biomolecular Crystallography

Presenting Author: David Moreau, Cornell University

Abstract Title: How to collect better data? Longer exposure times versus higher redundancy

Presenting Author: Michael Ruf, Bruker AXS Inc

Abstract Title: A simple technique to classify diffraction data from dynamic proteins according to individual polymorphs

Presenting Author: Alexei Soares, Brookhaven National Laboratory

Abstract Title: Rapid response to biomedical challenges and threats

Presenting Author: Wladek Minor, University of Virginia



4.2.3 Sample Prep for Cryo-EM and Crystallography

8/1/2021

Chair(s): Edward Pryor

Sponsoring SIG: Cryo EM

Co-Sponsoring SIG: Best Practices

With the technological advancements in both X-ray crystallography and Cryo-EM, structural biology techniques are becoming readily accessible to all labs. Although we are witnessing many significant strides in this field, preparation of high-quality samples still remains as one of the main bottleneck for both methods. In this session we will highlight the latest sample preparation methods, techniques, and best practices for both crystallography and Cryo-EM single particle, tomography, and micro-ED workflows.

Abstract Title: A Fab-ulous approach for solving structures of small membrane proteins using cryo-EM

Presenting Author: **Rosemary Cater, Columbia University**

Abstract Title: MicroED: conception, practice and future opportunities

Presenting Author: **Tamir Gonen, HHMI/UCLA**

Abstract Title: Sample preparation technologies for serial synchrotron crystallography and single-particle cryo-EM

Presenting Author: **Robert Thorne, MiTeGen, LLC**

Abstract Title: Novel Solutions to Accelerate Cryo-EM Single Particle Analysis Sample Screening

Presenting Author: **Atieh Aminian**

Abstract Title: TELSAM accelerates crystallization of fused target proteins by stabilizing weak crystal contacts

Presenting Author: **Supeshala Sarath Nawarathnage**

Abstract Title: Correlates of successful structure solution in cryoEM single particle reconstruction (SPR)

Presenting Author: **Dominika Borek, UT Southwestern Medical Center**

4.2.4 Self Assembly in Soft Matter Systems

8/4/2021

Chair(s): Tom Fitzgibbons & Volker Urban

Sponsoring SIG: SAS

Polymeric systems that are covalently bonded that exhibit poor compatibility will often self-assemble in ways to minimize the free energy of the system. This can occur in solution or through a drying process towards the solid state. The self assembled structures play a key role in many applications ranging from lithography in electronic materials and nano templating to drug delivery vehicles and emulsion



stabilization. Small angle X-ray and neutron scattering provide unique insight to the self assembled structures of block copolymers and amphiphilic. Advances in small angle scattering along with the accompanying modeling efforts have accelerated work in this field by providing insight into TH structures and phase transitions that occur in these systems. In this session, we will bring together experts in both experimental and modeling efforts associated with describing the self-assembly of polymeric systems and their associated phase transitions.

Abstract Title: Nano-scale Structure and Composition of Mixed Micelles Revealed by Small-Angle Neutron Scattering (SANS) and Molecular Dynamics (MD)

Presenting Author: Paschalis Alexandridis, University at Buffalo, The State University of New York (SUNY)

Abstract Title: Structural analysis of self-assembled block copolymer systems using small angle neutron and x-ray scattering techniques

Presenting Author: Changwoo Do, Oak Ridge National Laboratory

Abstract Title: Structural Studies on Soft Matter Self-Assembly with Small-Angle X-ray Scattering

Presenting Author: Xiaobing Zuo, Argonne National Laboratory

Abstract Title: Molecular packing in double gyroid cubic phases revealed via resonant soft X-ray scattering

Presenting Author: Chenhui Zhu, Lawrence Berkeley National Laboratory

Abstract Title: Controlling the Morphology of Lipid Bicelles

Presenting Author: Volker Urban, Oak Ridge National Laboratory

Abstract Title: Assemblies of DNA grafted nanoparticles deciphered by SAXS

Presenting Author: Byeongdu Lee, Argonne National Laboratory

Abstract Title: Polarized resonant soft X-ray scattering measurements in polymer-grafted nanoparticles

Presenting Author: Dean DeLongchamp, NIST

4.2.5 Structure-based drug design

8/2/2021

Chair(s): Anna Gardberg & Elizabeth Sprague & Hans-Peter Biemann

Sponsoring SIG: Industrial

Co-Sponsoring SIG: Bio

In this session we will feature applications of structural biology methods to drug discovery. Possible topics may include structure/function studies to inform drug discovery, hit validation, lead optimization challenges and fragments with a particular interest in examples involving a variety of techniques (e.g. x-



ray, NMR, EM, in silico, biophysics, etc.). Technology or methods development in these areas is also of interest.

Abstract Title: **Structure-Guided Design of Cryptococcus neoformans Protein Farnesyltransferase Inhibitors with Antifungal Activity**

Presenting Author: **You Wang, Duke University**

Abstract Title: **Ligand-induced global conformational changes in TBP-associated factor 1 (TAF1) tandem bromodomains – a novel strategy for targeting the TAF1.**

Presenting Author: **Md Rezaul Karim**

Abstract Title: **Cryo-EM structures of inhibitory antibodies complexed with Arginase1 provide insight into mechanism of action.**

Presenting Author: **Veronica Juan, Merck Research Labs**

Abstract Title: **Taking away PAIN: Enabling new structures of the Nav1.7 sodium channel by cryo-EM**

Presenting Author: **Christine Jao, Genentech**

Abstract Title: **Bispecifics and CAR T cells that target intracellular cancer driver mutations**

Presenting Author: **Sandra Gabelli, Johns Hopkins University**

Abstract Title: **Structure-Based Drug Design of Bcl-XL Selective Inhibitors**

Presenting Author: **Russell Judge, Structural Biology GPRD R467, AbbVie**

Abstract Title: **Fragments of stories**

Presenting Author: **Roderick Hubbard**

PL1 Etter Award

8/1/2021

Abstract Title: **How to discover new solids containing alkali metals: predictive screening, facile synthesis and in situ studies**

Presenting Author: **Julia Zaikina, Department of Chemistry Iowa State University**

PL2 Buerger Award

8/2/2021

Abstract Title: **CryoEM Structures of Macromolecules**

Presenting Author: **Wah Chiu, Department of Bioengineering, Stanford University, Stanford, CA, USA**



PL3 Warren Award

8/3/2021

Abstract Title: **Molecular Engineering of Single-crystal Optical Actuators**
Presenting Author: **Jacqueline Cole**

PS1 Poster Session I

7/31/2021

Chairs: Sara Andres & Leighanne Gallington

Abstract Title: **A glimpse at the Balch-Olmstead fullerene legacy**
Presenting Author: **Mrittika Roy, University of California, Davis**

Abstract Title: **A structural investigation into an alpha-mannosidase found in Bacteroides thetaiotaomicron**
Presenting Author: **Nicole Fraser, University of Waterloo**

Abstract Title: **Avoiding Sample Collisions with Puck Visualization for MX**
Presenting Author: **Samuel Clark, Hofstra University**

Abstract Title: **Biochemical analysis and review of the active site evolution of SARS-CoV-2 and other coronaviruses.**
Presenting Author: **Mickayla Bacorn**

Abstract Title: **Bioinformatics and 3D Structural Analysis of the Coronavirus Main Protease Active Site**
Presenting Author: **Amy Wu Wu, University of Puerto Rico, Mayagüez Campus**

Abstract Title: **Extraordinary Structures of Orphan Methyltransferases with Their Substrate DNA**
Presenting Author: **John Horton, MD Anderson Cancer Center of The University of Texas**

Abstract Title: **Factors of Atomic Electron Scattering (FAES): A resource for Gaussian parameterization of integral ionic, fractionally charged, and neutral electron scattering factors**
Presenting Author: **Ambarneil Saha, University of California, Los Angeles**

Abstract Title: **Magnetic behavior of Cu-intercalated MnPSe₃**
Presenting Author: **Mohamed Nawwar, The Ohio State University**

Abstract Title: **Operando oxidation and reduction neutron scattering studies on pristine and Pt-coated ceria nanorods**
Presenting Author: **Sreya Paladugu, The University of Tennessee, Knoxville**



Abstract Title: **Optimizing the conditions for GGDPs crystal growth**
Presenting Author: **Andrew Pham**

Abstract Title: **Porting Crystal Structure Data to Virtual Reality using CAD2VR**
Presenting Author: **Nichole Valdez, Sandia National Laboratories**

Abstract Title: **Structural basis of inhibition of the NUDIX family ORF141**
Presenting Author: **Maurice Bessman, Johns Hopkins University**

Abstract Title: **Structural Comparison of Faecalibacterium prausnitzii α -glycosidases and Sucrase-Isomaltase**
Presenting Author: **Anna Jewczynko, University of Waterloo**

Abstract Title: **Structural Insight into Replication Fidelity and Primer Shuttling in Human Mitochondrial DNA Polymerase Gamma**
Presenting Author: **Joon Park, University of Texas Medical Branch**

Abstract Title: **Structural insight into the neosubstrate selectivity of thalidomide metabolite**
Presenting Author: **Hirotake Furihata, The University of Tokyo**

Abstract Title: **Structural insights into the mechanisms of substrate recognition and catalysis for the N-methyltransferases involved in benzyloquinoline alkaloid metabolism**
Presenting Author: **Dean Lang**

Abstract Title: **Structural Studies of the Conjugative Entry Exclusion Protein from the F and R100 Plasmids, TraG**
Presenting Author: **Nicholas Bragagnolo, York University**

Abstract Title: **The role of BAM in mediating Fusobacterium nucleatum infection and pathogenesis**
Presenting Author: **Claire Overly, Purdue University**

Abstract Title: **Towards the structural analysis of an F plasmid protein, TraW**
Presenting Author: **Christina Rodriguez, York University**

Abstract Title: **Understanding the active site of the SARS-CoV-2 papain-like protease (PLPro)**
Presenting Author: **MaryAgnes Balogun, Morgan State University**

Abstract Title: **What is a single cryo-EM image worth? A survey of high-resolution cryo-EM model system datasets**
Presenting Author: **Vinh Truong**



PS2 Poster Session II

8/1/2021

Chairs: Sara Andres & Leighanne Gallington

Abstract Title: **A Zwitterionic Metal-Organic Framework for the Capture and Release of Iodine**

Presenting Author: **Charlene VanLeuven, Clarkson University**

Abstract Title: **Algebraic analysis of topological domain-interface defects in crystals**

Presenting Author: **James McKenzie**

Abstract Title: **B4 Autocollect: a Fully Automated Data Collection and Data Processing Pipeline at the Berkeley Center for Structural Biology**

Presenting Author: **Daniil Prigozhin, Lawrence Berkeley National Laboratory**

Abstract Title: **BioCAT beamline enables high quality equilibrium and time resolved biological solution SAXS**

Presenting Author: **Jesse Hopkins, BioCAT (Sector 18, APS), Illinois Institute of Technology**

Abstract Title: **Cryo-EM reveals that MuB is an AAA+ regulator of transposition that distorts target DNA**

Presenting Author: **Eshan Mehrotra, Cornell University**

Abstract Title: **Crystal Structure of a Zirconium Based Hydrogen Storage Material**

Presenting Author: **Nayeli Garcia, UNT Dallas**

Abstract Title: **Design and Characterization of Rare Earth Metal-Based Zwitterionic Metal-Organic Frameworks**

Presenting Author: **Kirti Sharma, Clarkson University**

Abstract Title: **Discover: A Total Scattering Diffractometer for Materials Discovery at the SNS**

Presenting Author: **Peter Metz, Oak Ridge National Laboratory**

Abstract Title: **Evaluation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model in an infinite crystal.**

Presenting Author: **Jessie Weatherly, Middle Tennessee State University**

Abstract Title: **Examining structural and magnetic preferences in elemental substitution on MnPSe₃**

Presenting Author: **Sogol Lotfi**

Abstract Title: **Insights into Benzylisoquinoline Alkaloid Recognition Revealed by the 2.4 Å... Crystal Structure of Codeionone Reductase**

Presenting Author: **Samuel Carr, University of Calgary**



Abstract Title: **Mg²⁺ and Mn²⁺ coordinate Cap-0-RNA to position substrates for efficient 2Å'-O-methyl transfer by SARS-CoV-2 nsp16**

Presenting Author: **George Minasov, 1Department of Microbiology-Immunology, Northwestern University, Chicago**

Abstract Title: **Micro crystal electron diffraction of the peptide Gramicidin**

Presenting Author: **Nicole Hoefer, The Ohio State University**

Abstract Title: **New Structural Insights into the Function of the Catalytically Active Human Taspase1**

Presenting Author: **Jose Martin-Garcia, Institute of Physical Chemistry Rocasolano, CSIC**

Abstract Title: **On the Completeness of Three-Dimensional Electron Diffraction Data for Structural Analysis of Metal-Organic Frameworks**

Presenting Author: **Meng Ge, Stockholm University**

Abstract Title: **PDB-101 Video Challenge: Creating a Winning Entry**

Presenting Author: **Ethan Cartagena**

Abstract Title: **Progress towards developing an experimental platform for high-throughput CryoSAXS**

Presenting Author: **David Moreau, Cornell University**

Abstract Title: **RCSB Protein Data Bank: Integrated Searching and Efficient Access to Macromolecular Structure Data from the PDB Archive**

Presenting Author: **Brian Hudson, RCSB Protein Data Bank**

Abstract Title: **Solid State Photoreactivity of Cinnamic Acid and Crotonic Acid Compared**

Presenting Author: **Mehdi Esmaili, University of Guelph**

Abstract Title: **Structure and function of the respiratory syncytial virus polymerase**

Presenting Author: **Bo Liang, SOM, Emory University**

Abstract Title: **Structure of RNA-dependent RNA Polymerase 2 (RDR2) and its implications for double-stranded RNA synthesis in gene silencing**

Presenting Author: **Yuichiro Takagi, Biochemistry & Molecular Biology, Indiana Univ School of Medicine**

Abstract Title: **The next generation RCSB.org**

Presenting Author: **Justin Flatt**

Abstract Title: **Trends in macromolecular structure data across 50 years of the PDB**

Presenting Author: **Yuhe Liang, RCSB Protein Data Bank**



Abstract Title: **Understanding the short-range magnetic correlations in MnTe through magnetic pair distribution function analysis**

Presenting Author: **Jacob Christensen, Brigham Young University**

Abstract Title: **Understanding the structural and functional details of Rv3716c, a hypothetical protein from Mycobacterium tuberculosis**

Presenting Author: **Geeta Deka, National Centre for Biological Sciences (NCBS), Bangalore**

Abstract Title: **Using data mining to identify variations within the proteases of Coronaviridae**

Presenting Author: **Cassandra Olivas, California State University, Stanislaus**

Abstract Title: **Zirconium Hydroxide: Towards Facile Room-Temperature Synthesis of Zr-based Metal-Organic Frameworks**

Presenting Author: **Yunzhuo Li**

PS3 Poster Session III

8/2/2021

Chairs: Sara Andres & Leighanne Gallington

Abstract Title: **A simple vapor-diffusion method enables protein crystallization inside the HARE serial crystallography chip**

Presenting Author: **Pedram Mehrabi, Max Planck Institute for the Structure and Dynamics of Matter**

Abstract Title: **Crystal Structure and Characterization of Human Heavy-Chain Only Antibodies Reveals a Novel, Stable Dimeric Structure Similar to Monoclonal Antibodies**

Presenting Author: **Soheila Bahmanjah, Merck**

Abstract Title: **Crystal Structures of Large-Volume Commercial Pharmaceuticals**

Presenting Author: **James Kaduk, Chemistry, Illinois Inst of Technology**

Abstract Title: **Electron cryo-microscopy at 100 and 200 kV: from screening to structures**

Presenting Author: **Dimple Karia, Materials and Structural Analysis Division Thermo Fisher Scientific Netherlands**

Abstract Title: **Elucidating lactate oxidase enzyme-biomarker lactate interactions by SAXS, crystallography and X-ray footprinting for developing a real-time stress biosensor.**

Presenting Author: **Rohit Jain, Case Western Reserve University**

Abstract Title: **Growing protein crystals under different conditions**

Presenting Author: **Andrej Arendt, Karl Popper Schule, Frankfurt**

Abstract Title: **Histone H4 acetyllysine coordination by ATAD2 bromodomain**

Presenting Author: **Margaret Phillips, Univeristy of Vermont**



Abstract Title: **Improving data quality for 3D electron diffraction (3DED) by Gatan Image Filter**
Presenting Author: **Taimin Yang, Stockholm University**

Abstract Title: **Innovations in Electric Field-Stimulated X-Ray Crystallography**
Presenting Author: **Jack Greisman, Harvard University**

Abstract Title: **Novel Cocrystallization of Apolipoprotein A-I with Butyric Acid**
Presenting Author: **Grace Ferri**

Abstract Title: **Pressure-induced reentrance of ferroelectricity in a molecular magnet**
Presenting Author: **Yan Wu, Oak Ridge National Lab**

Abstract Title: **Structural analysis of the Toc75 Potra domains from Pisum sativum**
Presenting Author: **Karthik Srinivasan, Purdue University**

Abstract Title: **Structural and functional characterization of the glycosyltransferase PglA from Campylobacter concisus**
Presenting Author: **Nemanja Vuksanovic**

Abstract Title: **Structural and functional studies on Salmonella typhimurium pyridoxal kinase: the first structural evidence for the formation of Schiff base with the substrate**
Presenting Author: **Geeta Deka, National Centre for Biological Sciences (NCBS), Bangalore**

Abstract Title: **Structural Characterization of the Homeodomain Transcription Factor Gsx2 Bound to DNA**
Presenting Author: **Jordan Webb, University of Cincinnati**

Abstract Title: **Structural Investigation of 4,4,8,8-Tetrahalotricyclo[5.1.0.0^{sup}3,5^{sup}]]octanes**
Presenting Author: **Kent Clinger**

Abstract Title: **Structural investigations into the avian MHC-I like protein YF1*7.1**
Presenting Author: **Yogesh Khandokar, The university of Melbourne**

Abstract Title: **The electron diffractometer: A dedicated user-friendly device for electron crystallography experiments**
Presenting Author: **Gustavo Santiso-Quinones, Eldico Scientific AG**

Abstract Title: **Two riboswitches with identical binding pockets and disparate RNA folds show different tolerances to equivalent mutations.**
Presenting Author: **Kumari Yoshita Srivastava, Department of Biophysics and Biochemistry, University of Rochester Medical Center**



Abstract Title: **Un[i]lox[/i]ing the assembly and activation mechanism of Cre recombinase using cryo-EM**

Presenting Author: **Kye Stachowski, The Ohio State University**

PS4 Poster Session IV

8/3/2021

Chairs: Sara Andres & Leighanne Gallington

Abstract Title: **A Compact Liquid Sample Automatic Handling System for Remote BioSAXS Operation**

Presenting Author: **Xiaobing Zuo, Argonne National Laboratory**

Abstract Title: **Advanced data collection at FMX – the Frontier Microfocusing Macromolecular Crystallography Beamline at the National Synchrotron Light Source II**

Presenting Author: **Martin Fuchs, Photon Sciences, Brookhaven National Lab**

Abstract Title: **AutoMicroED: A semi-automated MicroED processing pipeline**

Presenting Author: **Samantha Powell, Pacific Northwest National Lab**

Abstract Title: **BioMAX, a macromolecular crystallography facility at MAX IV**

Presenting Author: **Ana Gonzalez, MAX IV**

Abstract Title: **Crystal Structure of an Archaeal Dihydroorotase**

Presenting Author: **Jacqueline Vitali, Cleveland State University**

Abstract Title: **Developments in Advanced Handling, Storage, Transport, and Tracking of Cryo-EM Samples**

Presenting Author: **Benjamin Apker, MiTeGen**

Abstract Title: **Introducing the XtaLAB Synergy Flow**

Presenting Author: **Mark Del Campo, Life Sciences, Rigaku Americas Corporation**

Abstract Title: **Introducing undergraduate students to single crystal X-ray diffraction through a course-based undergraduate research experience**

Presenting Author: **Gregory McManus, Florida Gulf Coast University**

Abstract Title: **Learning in the Lockdown: Free Online CryoEM School**

Presenting Author: **Geoffrey Woollard**

Abstract Title: **Microgravity crystallization for improving uniformity and homogeneity of crystals for time-resolved diffusive mixing XFEL experiments**

Presenting Author: **Jason Stagno, Center for Structural Biology, Center for Cancer Research, National Cancer Institute**



Abstract Title: **Modeling and machine learning tools to improve image processing in crystallization screening**
Presenting Author: **Miranda Lynch, Hauptman-Woodward Medical Research Institute**

Abstract Title: **New Developments of Microfocus X-Ray Sealed Tube Sources for In-house Crystallography**
Presenting Author: **Joerg Wiesmann**

Abstract Title: **Scanning mapping of biological tissues using scattering contrast**
Presenting Author: **jiliang liu, ESRF**

Abstract Title: **Synergy-ED: A new electron diffractometer for microED**
Presenting Author: **Joseph Ferrara, Rigaku Americas Corp**

Abstract Title: **The Future of Co-crystallisation: A New Workflow Based on AI Predictions, the Crystal16 Platform and Electron Diffraction**
Presenting Author: **Carmen Guguta, Technobis Crystallization Systems**

Abstract Title: **THE NATIONAL CENTER FOR CRYOEM ACCESS AND TRAINING : NATIONWIDE ACCESS TO CRYOEM TECHNOLOGY AND CURRICULA**
Presenting Author: **Edward Eng, New York Structural Biology Center**

Abstract Title: **Transitioning from a crystallographer to a structural biologist: Lessons learned**
Presenting Author: **John Rose, SER-CAT/University of Georgia**

Abstract Title: **Understanding the structure of (1-x)BaZr0.2Ti0.8O3 - (x)Ba0.7Ca0.3TiO3 based lead-free piezoelectric materials**
Presenting Author: **Alicia Manjon Sanz, Oak Ridge National Laboratory**

TR1 Transactions: PDB 50th

7/30/2021

Chair(s): Stephen Burley & David Rose

Abstract Title: **Histone H2B ubiquitination in transcription regulation**
Presenting Author: **Cynthia Wolberger, Biophysics & Biophysics Chemistry, Johns Hopkins School Of Medicine**

Abstract Title: **Cryo-FIB Milling Improves MicroED Data and Structures**
Presenting Author: **Mike Martynowycz, HHMI/UCLA**

Abstract Title: **Macromolecular machines at energized membranes**
Presenting Author: **John Rubinstein, The Hospital for Sick Children**



Abstract Title: **Crystallographic snapshots of TsrM, a cobalamin-dependent radical S-adenosylmethionine methylase**

Presenting Author: **Squire Booker, Penn State, State College, PA**

Abstract Title: **Developing novel tools to guide the discovery of new cell-permeable, on-target anti-infective compounds.**

Presenting Author: **RAFAEL COUNAGO, UNICAMP**

Abstract Title: **A Global consortium, next-generation SARS-CoV-2 antibody therapeutics and stabilized spike**

Presenting Author: **Erica Sapphire**

TR2 Transactions: PDB 50th

7/31/2021

Chair(s): Stephen Burley & David Rose

Abstract Title: **Innovation by Evolution: Bringing New Chemistry to Life**

Presenting Author: **Frances Arnold, California Institute of Technology**

Abstract Title: **Reflections on Resolution and Revolution – the PDB and me**

Presenting Author: **Wayne A. Hendrickson, Columbia University**

Abstract Title: **Structural biology response to biomedical threats**

Presenting Author: **Wladek Minor, University of Virginia**

Abstract Title: **Protein folding computed from evolutionary information**

Presenting Author: **Chris Sander, Harvard Medical School**

Abstract Title: **Structural relationships between human transcriptional coactivators TFIID and SAGA**

Presenting Author: **Eva Nogales, UC Berkeley**

Abstract Title: **From integrative structural biology to cell biology**

Presenting Author: **Andrej Sali**



Workshops

<p>Monday, August 9, 2021 12:00 PM EST - 4:00 PM ET</p>	<p>WK2: Introduction to Hydroxyl Radical Footprinting Methods for Structural Analysis of Proteins and Complexes</p> <p>Primary Organizational Contact: Corie Ralston Head, Berkeley Center for Structural Biology, Molecular Biophysics & Integrated Bioimaging, Lawrence Berkeley National Laboratory Lawrence Berkeley Laboratory</p>
<p>Monday, August 9, 2021 1:00 PM EST - 5:00 PM ET (PART 1) Tuesday, August 10, 2021 1:00 PM EST - 5:00 PM ET (PART 2) Wednesday, August 11, 2021 1:00 PM EST - 5:00 PM ET (PART 3)</p>	<p>WK1: Characterization of Soft Materials Via Small Angle Scattering: Applications of Scattering for Polymer Systems</p> <p>Primary Organizational Contact: Thomas Fitzgibbons Research Scientist, Core R&D Dow Chemical</p> <p>Organizational Committee Member: Tyler Martin Polymer Processing Group NIST Jan Ilavsky Physicist, Beamline Scientist Argonne National Lab, XSD, 9-ID</p> <p>Instructor/Organizational Committee Member: Greg Beaucage Professor, Chemical and Materials Engineering University of Cincinnati</p> <p>Instructor/Organizational Committee Member: Lucia Fernandez-Ballester Assistant Professor, Mechanical and Materials Engineering University of Nebraska, Lincoln</p>
<p>Thursday, August 12, 2021 1:00 PM ET - 5:00 PM ET</p>	<p>WK5: MicroED of Small and Macromolecules</p> <p>Primary Organizational Contact: Tamir Gonen David Geffen School of Medicine at UCLA Department of Biological Chemistry Instructor/Organizational Meeting Committee Member Brandon Mercado Department of Chemistry, Yale University Chemical and Biophysical Instrumentation Center</p>



<p>Monday, August 16, 2021 12:00 PM ET - 6:00 PM ET</p> <p>*Optional Reception: August 18, 2021 6:00 PM ET *</p>	<p>WK4: Managing and Using National Cryo-EM Facilities</p> <p>Primary Organizer/Instructor Ed Eng, NYSBC/NCCAT</p> <p>Instructor Craig Yoshioka, PNCC</p> <p>Instructor Ulrich Baxa, NCEF</p> <p>Instructor Anchi Cheng, NYSBC/NCCAT</p> <p>Instructor Corey Hecksel, S2C2</p> <p>Instructor Sean Mulligan, PNCC</p> <p>Instructor Dmitry Tegunov, Max Planck Institute</p>
<p>Tuesday, August 17, 2021 12:00 PM ET - 6:00 PM ET (PART 1)</p> <p>Wednesday, August 18, 2021 12:00 PM ET - 6:00 PM ET (PART 2)</p> <p>*Optional Reception: August 18, 2021 6:00 PM ET *</p>	<p>WK3: Fundamentals of Single Particle Cryo-EM</p> <p>Primary Organizational Contact: Mark Herzik, UC San Diego</p> <p>Instructor/Organizational Meeting Committee Member Elizabeth (Liz) Kellogg, Cornell</p> <p>Instructor/Organizational Meeting Committee Member Edward (Ed) Twomey, Johns Hopkins</p> <p>Instructor Eva Nogales, UC Berkley</p> <p>Instructor Edoardo D’Imprima, EMBL</p> <p>Instructor Michael Cianfrocco, U Michigan</p> <p>Instructor Chi-Min (Mimi) Ho, Columbia</p> <p>Instructor Oliver (Oli) Clarke, Columbia</p> <p>Instructor Ed Eng, NYSBC/NCCAT</p> <p>Instructor Craig Yoshioka, PNCC</p>

