ACA 2022
PORTLAND

ACA: The Structural Science Society
www.amercrystalassn.org

2022 Full Program w/ Abstract List

2022 ACA Meeting Committee:
C. Slebodnick
B. Mercado
A. Gardberg
S. Powell

Scientific sessions and workshops at the 2022 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.amercrystalassn.org/past-meetings.

If there is an abstract that you would like to view please go to here: https://www.amercrystalassn.org/past-meetings, click on the abstracts for the 2022 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#/).

Workshops

Workshop 1: Applications of Small Angle Scattering to Structural Biology: An Introduction
Organizational Contact: Michal Hammel

Workshop 2: X-ray and Cryo-EM structure determination with AlphaFold and Phenix
Organizational Contact: Dorothee Liebschner

Workshop 3: Cryo-Electron Tomography: State of the Art Methods
Organizational Contact: JT Kaelber

Workshop 4: Hands-on Single-Particle Cryo-EM Data Analysis with cryoEDU
Organizational Contact: Michael Cianfrocco, Ph.D.

Workshop 5: CryoEM sample preparation training using center merit badges

Organizational Contact: Ed Eng

Workshop 6: Advanced Software Tools for Single Crystal Diffraction
Organizational Contact: Xiaoping Wang

Workshop 7: Visualizing Structure
Organizational Contact: Nichole Valdez

Workshop 8: Microcrystal Electron Diffraction (MicroED)
Organizational Contact: Tamir Gonen, Jessica Bruhn

Saturday, July 30, 2022

TR1 The Role of Structural Science in Tackling a Pandemic: COVID-19 as a Paradigm

7/30/2022 @ 8:30:00 AM - 11:30:00 AM | Salon E
Session Chair(s): Diana Tomchick

Abstract Title: **Structural insights into 2'-O ribosyl methylation of mRNA cap by SARS-CoV-2**
Presenting Author: **Yogesh Gupta, University of Texas Health Science Center San Antonio**

Abstract Title: **The evolutionary arms race between antibody-mediated immunity and SARS-CoV-2**
Presenting Author: **Timothy Bates, Oregon Health & Science University**

Abstract Title: **Molecular mechanisms of COVID-19**
Presenting Author: **Fang Li, University of Minnesota**

Abstract Title: **Structural Biology Response to Biomedical Threats**
Presenting Author: **Wladek Minor, University of Virginia**

1.1.1 Emergent Phenomena Through High Pressure, Low Temperature, High Field & Other Extreme Conditions

7/30/2022 @ 8:30:00 AM - 11:30:00 AM | Salons C-D
Sponsoring SIG(s): Neutrons/Materials/Powder
Session Chair(s): Yue Meng; Bianca Haberl

The application of extreme conditions enables access to exotic states of matter. Under extremes, matter undergoes drastic changes such as structural and magnetic phase transitions or exhibits rich new phenomena such as novel superconductivity. The application of extremes also enables synthesis of new exotic materials with unique characteristics. Furthermore, extremes can also be used as 'tuning' parameters that can be used control and understand the quantum dynamics of strongly correlated electrons. In common to these research directions is the requirement to successful apply the desired (multi-)extreme conditions as well as characterization techniques that enable in situ study of materials while under extremes.

This session will address the many behaviors and phenomena that are observed under extreme conditions as well as necessary experimental and theoretical techniques. This session thus aims to bring together researchers reporting on the most recent experimental and theoretical discoveries of novel emergent phenomena as well as researchers targeting development and advancement of new techniques and approaches. Additional attention will be paid to existing and new capabilities at large-scale facilities world-wide. Finally, it will also provide a platform to exchange ideas to expand the scope of future materials research under extreme conditions

Abstract Title: **Tuning magnetism with pressure in honeycomb and square lattice Iridates**
Presenting Author: **Daniel Haskel, Argonne National Laboratory**

Abstract Title: **Magnetism in the bucked honey-comb lattice of Eu2Mg3Bi4**
Presenting Author: **Ranuri Dissanayaka Mudiyanselage, Rutgers University**

Abstract Title: **The magnetic and crystal symmetries of EuCd2As2 and their role in generating a single pair of Weyl points**
Presenting Author: **Keith Taddei, Oak Ridge National Lab**

Abstract Title: **Large volume press program at 16-BM-B: experimentally linking atomic structure and emergent macroscopic properties at high pressures and temperatures**
Presenting Author: **Rostislav Hrubiak, ANL**

Abstract Title: **Discovery of High Pressure Co-Bi Materials**
Presenting Author: **Catherine Badding, Massachussetts Institute of Technology**

Abstract Title: **Evidence for pressure-induced unconventional quantum criticality in the coupled spin-ladder antiferromagnet C9H18N2CuBr4**
Presenting Author: **Tao Hong, Neutron Scattering Division, Oak Ridge National Laboratory**

Abstract Title: **Pressure & Field: The keys to unlock exotic states in quantum materials**
Presenting Author: **Sara Haravifard, Duke University**

1.1.2 Use of AI predicted Models in Structural Biology/Crystallography

7/30/2022 @ 8:30:00 AM - 11:30:00 AM | Salon F
Sponsoring SIG(s): BioMac & Best Practices
Co-Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Aaron Brewster; John Moult

Prediction of 3D protein structure by AlphaFold2 and RoseTTAFold has achieved revolutionary accuracy using new AI methods. These programs can accurately predict the 3D structure of many proteins from 1D amino acid sequences, opening up a vast array of exciting new experiments and challenges for researchers. In this session we will explore current applications of these structures in molecular replacement, cryo-EM fitting and refinement, structure-based drug design, and tomography. We will explore what kinds of new and difficult methods have been enabled and what remains difficult. Other topics may include how error estimates on AI protein models can be incorporated into these methods, progress in modeling of protein complexes, implications of AI structures on protein design, the generation and use of structure ensembles, and new data analysis best practices that need to be developed as the use of computer-generated structures becomes more common.

Abstract Title: **Efficient and accurate prediction of protein structures and interactions using RoseTTAFold**
Presenting Author: **Minkyung Baek, University of Washington**

Abstract Title: **Assessing AlphaFold predictions**
Presenting Author: **Kathryn Tunyasuvunakool**

Abstract Title: **AlphaFold changes everything (and nothing)**
Presenting Author: **Thomas Terwilliger, New Mexico Consortium**

Abstract Title: **Use and Limitations of AlphaFold2 in the Structural Modeling of E3 Ubiquitin Ligase Tom1/HUWE1**

Presenting Author: **Jennifer Madrigal, University of Utah**

Abstract Title: **Unravelling the molecular architecture of the Commander assembly**
Presenting Author: **Michael Healy, Institute for molecular biosciences**

Abstract Title: **Assessing Macromolecular Crystal Structures for Agreement with Experimental Data at the Individual Amino Acid Residue Level**
Presenting Author: **Stephen Burley, RCSB Protein Data Bank, Rutgers University**

1.1.3 New Developments in cryoEM and cryoET: Towards Atomic Resolution

7/30/2022 @ 8:30:00 AM - 11:30:00 AM | Salons G-I
Sponsoring SIG(s): cryo-EM
Session Chair(s): Mark Herzik; Oliver Clarke

Single-particle cryogenic electron microscopy (cryoEM) and tomography (cryoET) can provide remarkable insights into the structure of macromolecules in either purified form or in a cellular context, respectively. Due to advances in direct electron detector technologies and algorithm developments over the past decade, cryoEM analysis can now routinely determine structures at resolution ranges previously deemed accessible only to X-ray crystallography (2-4Å), while cryoET has moved into the sub-nanometer range. However, ultra-high-resolution structures, where individual atoms are resolved, remained only accessible by crystallographic analysis until recently. Now, with the advent of new EM hardware, including more coherent electron sources, improved energy filters and more, cryoEM analysis is able to reach atomic resolution in favorable cases. In parallel, improvement in data collection methods and reconstruction approaches has allowed cryoET to similarly break new ground, with sub-3Å reconstructions now achievable. This session highlights both the technical developments that have allowed such advances, and the biological insights facilitated by improved structural resolution obtained by both cryoEM and cryoET.

Abstract Title: **Near-atomic level insights into the gap junctions resolved by CryoEM**
Presenting Author: **Steve Reichow, Portland State University**

Abstract Title: **Harnessing the power of cryo-EM for development of cancer therapeutics: High-resolution structures of the human CDK-activating kinase bound to inhibitors**
Presenting Author: **Basil Greber, Cancer Research, Chester Beatty Laboratories**

Abstract Title: **RELION 4 and beyond - Structural heterogeneity and algorithmic robustness**
Presenting Author: **Dari Kimanius**

Abstract Title: **Novel designed rigidified imaging scaffolds for high-resolution structure determination of small proteins with cryo-EM**
Presenting Author: **Roger Castells Graells, University of California Los Angeles**

Abstract Title: **Structural Parasitology of Malaria Parasites**
Presenting Author: **Chi-Min Ho, Columbia University Irving Medical Center**

Abstract Title: **Breaking down the barriers in cryo-EM analysis of membrane proteins**
Presenting Author: **Xiao Fan, Princeton University**

Abstract Title: **CRYOEM ANALYSIS OF GATING DYNAMICS IN MAMMALIAN BESTROPHINS**
Presenting Author: **Tingting Yang, Columbia University**

Abstract Title: **Industry Applications of Cryo-Electron Microscopy**
Presenting Author: **Nicole Poweleit, NanoImaging**

1.1.4 MicroED of small and macromolecules

7/30/2022 @ 8:30:00 AM - 11:30:00 AM | Salons A-B
Sponsoring SIG(s): Small Molecule
Session Chair(s): Tamir Gonen; Jessica Bruhn

The field of microcrystal electron diffraction (MicroED) has rapidly progressed in recent years bringing exciting new opportunities to the structural biology and analytical chemistry fields. This technique has been applied to a wide range of samples, from small molecules to peptides, to soluble proteins and even membrane proteins. Several experimental protocols exist that describe the process of sequentially recording diffraction patterns from nanometer-sized crystals while the crystal is continuously rotated in a transmission electron microscope and then using these data to determine 3D structures. This session will focus on method development with emphasis on advances in sample preparation, data collection software/hardware and data processing. This session will also provide an opportunity to highlight interesting recent applications of MicroED, especially for macromolecules and membrane proteins.

Abstract Title: **Quo Vadis MicroED?**
Presenting Author: **Tamir Gonen, HHMI/UCLA**

Abstract Title: **Revealing Structural Details with 3D Electron Diffraction/Microcrystal Electron Diffraction**
Presenting Author: **Jungyoun Cho, Stockholm University**

Abstract Title: **Tools for MicroED within the DIALS package**
Presenting Author: **David Waterman, STFC**

Abstract Title: **High resolution Micro-Electron Diffraction of protein crystals with Falcon 4(i)**
Presenting Author: **Abhay Kotecha, THERMO FISHER SCIENTIFIC**

Abstract Title: **MicroED workflow implementation in Leginon**
Presenting Author: **Anchi Cheng**

Abstract Title: **XtaLAB Synergy-ED: Over 160 Structures and Counting**
Presenting Author: **Joseph Ferrara, Rigaku Americas Corp**

Abstract Title: **MicroED of membrane proteins**
Presenting Author: **Anna Shiriaeva**

Abstract Title: **MicroED structure of Aeropyrum pernix protoglobin**
Presenting Author: **Emma Danelius, UCLA**

TMT 3-Minute-Thesis

7/30/2022 @ 11:30:00 AM - 1:00:00 PM | Salon F
Sponsoring SIG(s): YSIG
Session Chair(s): Dan Decato; Kristofer Gonzalez-DeWhitt

Abstract Title: **An autoregulation of DNA binding model of ZNF410 revealed by biophysical study of small-angle X-ray scattering**
Presenting Author: **Gundeep Kaur, MD ANDERSON CANCER CENTER**

Abstract Title: **Analysis of Primary Citations (References) of PDB Deposits**
Presenting Author: **Joanna Lenkiewicz, University of Virginia**

Abstract Title: **Capsid structure of a densovirus causing mass mortality in larval darkling beetles (Zophobas morio)**
Presenting Author: Judit Penzes, Rutgers University

Abstract Title: **Cryo-EM Structure of Pre-liganded NAIP5 reveals activation mechanism of NAIP/NLRC4 Inflammasome**
Presenting Author: **Bhaskar Paidimuddala, Oregon Health and Science University**

Abstract Title: **Defining the structural basis of ASCC2â€™s specificity for K63-linked polyubiquitin chains using 3D NMR analysis**
Presenting Author: **Rita Anoh, Mount St. Mary's University**

Abstract Title: **Novel designed rigidified imaging scaffolds for high-resolution structure determination of small proteins with cryo-EM**
Presenting Author: **Roger Castells Graells, University of California Los Angeles**

Abstract Title: **Structural insight into the transferrin-iron import system from pathogenicÂ Neisseria**
Presenting Author: **Shubham Dubey, Purdue University**

Abstract Title: **Structure of LiYbSe2 and Magnetism in a Pyrochlore Lattice**
Presenting Author: **Ranuri Dissanayaka Mudiyanselage, Rutgers University**

Abstract Title: **Two riboswitches that share a common ligand-binding fold show dramatic differences in the ability to accommodate mutations**
Presenting Author: **Kumari Yoshita Srivastava, Department of Biophysics and Biochemistry, University of Rochester Medical Center**

Abstract Title: **Understanding the role of pyridoxal reductase (PDXI) in pyridoxal 5â€™-phosphate (PLP) homeostasis.**
Presenting Author: **Akua Donkor, Virginia Commonwealth University**

Abstract Title: **UV related cataract formation: insights from serial synchrotron crystallography**
Presenting Author: **Jake Hill, University of Bradford**

Abstract Title: **Viral RNA Dependent RNA Polymerase forms Amyloids Like Fibrils via Liquid-Liquid Phase Separation**
Presenting Author: **Soni Kaundal, Baylor College of Medicine, Houston**

Abstract Title: **X-Ray Crystallography as a Tool to Understand the Structure-Property Relationship in Metal-Organic Frameworks for the Synthesis of Desired Sensor Materials**
Presenting Author: **Alisha Gogia, New Mexico Highlands University**

PL1 Etter Award:

Brent L. Nannenga
7/30/2022 @ 1:00:00 PM - 2:00:00 PM | Salon E

Abstract Title: **Microcrystal Electron Diffraction (MicroED) Methods and Applications**
Presenting Author: **Brent Nannenga, Arizona State University**

TR2 The Role of Structural Science in Tackling a Pandemic: COVID-19 as a Paradigm

7/30/2022 @ 2:00:00 PM - 5:00:00 PM | Salon E
Session Chair(s): Diana Tomchick

Abstract Title: **Creating new inhibitors to SARS-CoV-2 Macrodomain using Fragments, Neutrons, and Entropy!**
Presenting Author: **James Fraser, University of California, San Francisco**

Abstract Title: **Utilization of FIB-SEM Nanotomography to Visualize Early HCoV-229E Virus Mediated Endocytosis Nanoscale Interactions**
Presenting Author: **Alyssa Williams, McMaster University**

1.2.1 Structural Insights Into the Origin & Applications of Novel Properties in Quantum Materials

7/30/2022 @ 2:00:00 PM - 5:00:00 PM | Salons G-I
Sponsoring SIG(s): Neutrons/Materials/Powder
Session Chair(s): Keith Taddei; Haoxiang Li

Abstract Title: **Structure of LiYbSe2 and Magnetism in a Pyrochlore Lattice**
Presenting Author: **Ranuri Dissanayaka Mudiyanselage, Rutgers University**

Abstract Title: **Correlation between local symmetry breaking, magnetism and Weyl properties in Co3Sn2S2**
Presenting Author: **Qiang ZHANG**

Abstract Title: **Site Mixing and complex magnetic structures in topological insulators MnBi[sub]2[/sub]Te[sub]4[/sub] and MnSb[sub]2[/sub]Te[sub]4[/sub]**
Presenting Author: **Yaohua Liu, Oak Ridge National Laboratory**

Abstract Title: **Limiting Group Symmetry to Distinguish Non-toroidal, Ferrotoroidal, and Antiferrotoroidal Point Groups**
Presenting Author: **Stephanie Gnewuch, University of Maryland, College Park**

Abstract Title: **Study on transition metal chalcogenide intercalation chemistry through in-situ X-ray diffraction**
Presenting Author: **Huafei Zheng, University of Maryland, College Park Hyattsville, MD**

Abstract Title: **Structure Analysis of Metal-Chalcophosphate Layered Systems Using Micro-ED**
Presenting Author: **Anahita Pakzad**

1.2.3 Beamline Automation and Autonomous Experiments (II)

7/30/2022 @ 2:00:00 PM - 5:00:00 PM | Salons C-D
Sponsoring SIG(s): Light Sources
Session Chair(s): Masaki Yamamoto; Jean Jakoncic

With the technological advancements in automation at both synchrotron beamlines and sample handling, Macromolecular Crystallography (MX) has become an indispensable method for high-resolution structure analysis of biological macromolecules. In order to tackle the most challenging projects for modern life science and drug discovery research, the developments of further automation of MX and data analysis methods using high performance computing (HPC) to derive advanced structural information from large-scale diffraction data obtained by the automation are underway. A lot of results have been obtained by automated and remote data collection even in the global movement restrictions due to the COVID-19 pandemic. In this session we will highlight the latest automated sample handling and data collection methods, techniques, and best practices for advanced data analysis from large-scale diffraction data with automation.

Abstract Title: **Massif-1 at MASSIF-1 and fragment based drug design**
Presenting Author: **Didier Nurizzo**

Abstract Title: **Development of automated high-throughput MX beamline at SPring-8**
Presenting Author: **Masaki Yamamoto, Life Science Research Infrastructure Group, RIKEN SPring-8 Center**

Abstract Title: **Automation of X-ray Diffraction Data Analysis at SSRL**
Presenting Author: **Artem Lyubimov, Stanford Synchrotron Radiation Lightsource**

Abstract Title: **Automation at the Automated Macromolecular Crystallography (AMX) beamline at NSLS-II**
Presenting Author: **Dale Kreitler, National Synchrotron Light Source II**

Abstract Title: **Operation of a Versatile Compound Refractive Lens (CRL) Transfocator**
Presenting Author: **DAVID KISSICK, Argonne national laboratory Lemont, IL**

1.2.4 Machine Learning in cryo-EM

7/30/2022 @ 2:00:00 PM - 5:00:00 PM | Salon F
Sponsoring SIG(s): cryo-EM
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Joey Davis; Alexis Rohou

Powerful machine learning approaches have begun impacting cryo-EM and cryo-ET workflows in areas spanning data collection to reconstruction and model building. In many instances, these approaches are proving effective in automating labor-intensive tasks and in extracting information from the large, but low-signal datasets that electron microscopy typically produces. Additionally, careful application of these methods offers an opportunity to naturally encode prior structural information into the data analysis pipeline. When misapplied, however, the risk of introducing difficult-to-identify artifacts is significant, and robust validation methods are needed. This session features recent advances in machine learning methods and their applications to electron microscopy; highlighting the strengths, future prospects, and potential concerns of such approaches.

Abstract Title: **A Paradigm Shift in Structural Biology**
Presenting Author: **Sriram Subramaniam, UBC: The University of British Columbia VANCOUVER, BC**

Abstract Title: **Extracting free-energy profiles from cryo-electron microscopy experiments**
Presenting Author: **Pilar Cossio**

Abstract Title: **CryoRL: Reinforcement Learning Enables Efficient Cryo-EM Data Collection**
Presenting Author: **Michael Cianfrocco, University of Michigan**

Abstract Title: **TomoDRGN: resolving heterogeneous protein complexes in situ using cryo-ET and deep learning**
Presenting Author: **Barrett Powell, MIT**

Abstract Title: **CryoAI: Amortized Inference of Poses for Ab Initio Reconstruction of 3D Molecular Volumes from Experimental Cryo-EM Images.**
Presenting Author: **Frederic POITEVIN, SLAC National Accelerator Laboratory**

Abstract Title: **The continual learning and knowledge accumulation in cryoEM particle identification**
Presenting Author: **Xueming Li, Tsinghua University Beijing**

1.2.5 General Interest 1

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salons A-B
Sponsoring SIG(s): General Interest
Session Chair(s): Victoria Drago: Alexander Erickson; Elizaveta Katorcha

Abstract Title: **Structural Mining of Gut Metagenomes Pinpoints Therapeutically Relevant Microbial Enzymes**
Presenting Author: **Joshua Simpson, UNC Chapel Hill**

Abstract Title: **Reading the message: A structural and functional comparison of the ATAD2/B bromodomain binding activity**
Presenting Author: **Karen Glass, University of Vermont, Pharmacology Department Burlington, VT**

Abstract Title: **Structural and biochemical characterization of an interferon-inducible GTPase, human guanylate binding protein 2 (GBP2)**
Presenting Author: **Sayantan Roy, Florida State University**

Abstract Title: **Pentameric assembly of the Kv2.1 tetramerization domain**
Presenting Author: **Zhen Xu, the University of Iowa**

Abstract Title: **Towards a Structural and Atomic Mechanism for NIS Synthetase DesD: Laying the Groundwork for Structure-Based Drug Design.**
Presenting Author: **Katherine Hoffmann, California Lutheran University**

Abstract Title: **Making DC7 Invertible**

Presenting Author: **Herbert Bernstein, Ronin Institute for Independent Scholarship, c/o NSLS-II, Brookhaven National Lab, Bldg 745**

Abstract Title: **Cryo-EM structures reveal dramatic remodeling of the p97 hexamer by the multi-domain adapter UBXD1**
Presenting Author: **Julian Braxton, University of California, San Francisco**

1.3.1 John Spence Memorial Session

7/30/2022 @ 7:30:00 PM - 9:00:00 PM | Salon E
Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Rick Kirian

John Charles Howorth Spence (21 April 1946 – 28 June 2021) was Richard Snell Professor of Physics at Arizona State University and Director of Science at the National Science Foundation BioXFEL Science and Technology Center. He was endlessly fascinated by microscopy techniques and their applications in materials science (e.g. atomic-resolution electron microscopy and its use for the study of atomic defects in crystals and semiconductors) and molecular biology (e.g. x-ray imaging and crystallography techniques for imaging protein dynamics). He was a world-class inventor who tirelessly pursued truly unique and original ideas. He supported and inspired countless students, postdocs and colleagues along the way. Among many accolades, he was a Fellow of the National Academy of Inventors, honorary Fellow of the Royal Microscopical Society, Foreign Member of the Royal Society, and was awarded the Gregori Aminoff Prize in 2021. John's interests extend to music, literature, book-writing, flying, and sailing. He was an accomplished player of the piano, guitar and the flute and has been involved in many bands throughout the years. His most recent books published include "Lightspeed: The Ghostly Aether and the Race to Measure the Speed of Light" and "Spitfire Pilot Lou Spence: A Story of Bravery, Leadership and Love". Talks in this symposium will focus on various aspects of John's later years of work related to XFEL science and his pioneering contributions to the development of Serial Femtosecond Crystallography (see also the related symposium dedicated to John Spence at M&M - P12 on this website: https://www.microscopy.org/MandM/2022/program/descriptions.cfm.

Abstract Title: **John Spence and his interests in coherent imaging**
Presenting Author: **Henry Chapman, CFEL**

Abstract Title: **Where John Spence’s legacy leads us to: From static pictures to dynamics of biomolecules in action**
Presenting Author: **Petra Fromme, Arizona State University**

Abstract Title: **Convergent beam X-ray diffraction using multilayer Laue lenses An exploration following in John's footsteps**
Presenting Author: **,**

Abstract Title: **John Spence on a personal note**
Presenting Author: **Nadia Zatsepin, La Trobe University**

PS1 POSTER SESSION 1

7/30/2022 @ 5:30:00 PM - 7:30:00 PM
Exhibit Hall

Abstract Title: **A comprehensive strategy for quick determination of protein structures by MR-native SAD method**
Presenting Author: **Miki Senda, High Energy Accelerator Research Organization (KEK)**

Abstract Title: **An autoregulation of DNA binding model of ZNF410 revealed by biophysical study of small-angle X-ray scattering**
Presenting Author: **Gundeep Kaur, MD ANDERSON CANCER CENTER**

Abstract Title: **Analysis of Primary Citations (References) of PDB Deposits**
Presenting Author: **Joanna Lenkiewicz, University of Virginia**

Abstract Title: **Arrangement of Molecules for Photoreactions in Layered Peptide Crystals**
Presenting Author: **Mehdi Esmaeili, University of Guelph**

Abstract Title: **Conformational dynamics in modular enzyme systems studied by SAXS and cryo-EM**
Presenting Author: **Maxwell Watkins**

Abstract Title: **Cryo-EM Sample Preparation of native Myosin Filament from Striated Muscle**
Presenting Author: **Hosna Rastegarpouyani, Florida State University**

Abstract Title: **Cryo-EM Structure of Pre-liganded NAIP5 reveals activation mechanism of NAIP/NLRC4 Inflammasome**
Presenting Author: **Bhaskar Paidimuddala, Oregon Health and Science University**

Abstract Title: **Crystallographic analysis of hydrazine coordination modes with dichlorotris(triphenylphosphine)ruthenium(II)**

Presenting Author: **Kamran Ghiassi, Air Force Research Laboratory**

Abstract Title: **Dare to spin â€“ well diffracting protein nanocrystals through on-vortex crystallisation**
Presenting Author: **Gerhard Hofer, Stockholm University**

Abstract Title: **Defining the structural basis of ASCC2â€™s specificity for K63-linked polyubiquitin chains using 3D NMR analysis**
Presenting Author: **Rita Anoh, Mount St. Mary's University**

Abstract Title: **Elucidation of the Geometric Properties of the Pdu Microcompartment by Cryo-Electron Tomography**
Presenting Author: **Kevin Cannon, UCLA**

Abstract Title: **Enabling structure-based drug discovery for NUAK kinases**
Presenting Author: **Robert Hayes, Merck**

Abstract Title: **Fixed-Targets for Serial Protein Crystallography at SwissFEL**
Presenting Author: **Melissa Carrillo**

Abstract Title: **In situ architecture of the human kinetochore visualized by cryo-electron tomography**
Presenting Author: **WEI ZHAO, California Institute of Technology**

Abstract Title: **Integrative Modeling of the ASCC2:K63Ub2 Complex to Better Understand DNA Alkylation Damage Repair**
Presenting Author: **Zachary Beck, Mount St. Mary's University**

Abstract Title: **KHNYN is a Zinc-Finger Antiviral Protein (ZAP) co-factor that degrades ZAP-bound RNA**
Presenting Author: **Jennifer Meagher, University of Michigan**

Abstract Title: **Microgravity Crystallization and Neutron Diffraction of Perdeuterated Tryptophan Synthase**
Presenting Author: **Victoria Drago, Oak Ridge National Laboratory**

Abstract Title: **New Opportunities for Structural Biology Research at LCLS and SSRL**
Presenting Author: **Darya Marchany-Rivera, SLAC/SSRL-SMB**

Abstract Title: **Radiolytic Damage in Small-Molecule 3D Electron Crystallography**
Presenting Author: **Ambarneil Saha, University of California, Los Angeles**

Abstract Title: **Structural and Enzymatic Comparison of Faecalibacterium prausnitzii GH31 Î±-glycosidases**
Presenting Author: **Anna Jewczynko, University of Waterloo**

Abstract Title: **Structural Dynamics of Non-Ribosomal Peptide Synthetases**
Presenting Author: **Jitendra Singh, University at Buffalo**

Abstract Title: **Structure determination of novel quantum spin liquid crystal at NSFâ€™s ChemMatCARS**
Presenting Author: **Tieyan Chang, The University of Chicago**

Abstract Title: **Sub-100 Microsecond Time Resolved SAXS at BioCAT**
Presenting Author: **Jesse Hopkins, BioCAT (Sector 18, APS), Illinois Institute of Technology**

Abstract Title: **The enzyme EryM gives a helping hand in natural product biosynthesis**
Presenting Author: **Yihua Li, University of Michigan**

Abstract Title: **Time-resolved and Multi-temperature Crystallography of PEPCK Allows Observation of Previously Unobserved Dynamics and Structural States**
Presenting Author: **Jonathan Clinger, Cornell University**

Abstract Title: **Towards solving the hydrogenase maturation mystery**
Presenting Author: **Parag Gajjar, Brigham Young University**

Abstract Title: **Two riboswitches that share a common ligand-binding fold show dramatic differences in the ability to accommodate mutations**
Presenting Author: **Kumari Yoshita Srivastava, Department of Biophysics and Biochemistry, University of Rochester Medical Center**

Abstract Title: **Tying the knot in the tetrahydrofolate (THF) riboswitch: A molecular basis for gene regulation**
Presenting Author: **Jason Stagno, Center for Structural Biology, Center for Cancer Research, National Cancer Institute**

Abstract Title: **Understanding substrate binding and delivery through the bi-chaperone Hsp104_Hsp70 supercomplex**
Presenting Author: **Alexandrea Rizo**

Abstract Title: **Using Structural Biology to Elucidate Differences in Kinetic Inhibition Data Between Different Isozymes of PEPCK**
Presenting Author: **Sarah Barwell, University of Waterloo**

Abstract Title: **UV related cataract formation: insights from serial synchrotron crystallography**
Presenting Author: **Jake Hill, University of Bradford**

Abstract Title: **X-Ray Crystallography as a Tool to Understand the Structure-Property Relationship in Metal-Organic Frameworks for the Synthesis of Desired Sensor Materials**
Presenting Author: **Alisha Gogia, New Mexico Highlands University**

Abstract Title: **A Room temperature Polar and Weak-ferromagnetic Oxide with Low Dielectric Loss**
Presenting Author: **Nagamalleswari Katragadda, SRM University AP**

Abstract Title: **Characterization of a Trifunctional Sulfate-Activating Complex from Mycobacteria**
Presenting Author: **Samantha Hartanto, Department of Chemistry, University of California Davis**

YMIX YSIG mixer: The Hotel Zags

7/30/2022 @ 7:00:00 PM - 9:00:00 PM
Session Chair(s): Kenny Childers; Kristofer Gonzalez-DeWhitt

Sunday, July 31, 2022

2.1.1 New Developments for Operando and In Situ Diffraction

7/31/2022 @ 8:30:00 AM - 11:30:00 AM | Salons C-D
Sponsoring SIG(s): Neutrons/Materials/Powder
Session Chair(s): Jue Liu; Rebecca McAuliffe

Rational design of new functional solid state materials requires an atomistic understanding of reaction mechanisms during synthesis. To optimize the performance of these functional materials, monitoring the structural evolution of materials during device operation is key. In situ and operando X-ray/neutron diffraction have emerged as one of the most important characterization tools to study these chemical processes. The tremendous advancements of X-ray and neutron sources in recent years, together with improved instrument design, data acquisition and analysis enabled the unprecedent speed of diffraction data collection, on-the-fly data analysis and quantitative structure analysis of large amounts of data sets. Thus, we feel it is timely and imperative to highlight some of these exciting progresses and provide a platform to exchange ideas about future directions.

This symposium invites contributions from technique/instrumentation developments, advanced data analysis and scientific applications for operando and in situ X-ray/neutron diffraction.

Abstract Title: **High energy synchrotron powder diffraction beamlines for in situ and operando experiments: status, opportunities and challenges**
Presenting Author: **Wenqian Xu**

Abstract Title: **Beamline-like capabilities for in-situ X-ray diffraction work using modern in-house instrumentation**
Presenting Author: **Chris Malliakas, Northwestern University**

Abstract Title: **Opportunities and Challenges for In Situ Synchrotron Characterization of All Solid State Batteries**
Presenting Author: **Marm Dixit, Oak Ridge National Laboratory**

Abstract Title: **Designing next generation emissions abatement catalysts using operando neutron total scattering**
Presenting Author: **Sreya Paladugu, The University of Tennessee, Knoxville**

Abstract Title: **In situ X-ray diffraction studies of reaction heterogeneity in rechargeable batteries**
Presenting Author: **Hao Liu, Binghamton University**

Abstract Title: **In-situ high temperature spatially resolved X-ray diffraction of TiB2 up to ~3250 ËšC**
Presenting Author: **Scott McCormack, University of Californa, Davis**

2.1.2 Advances in Fiber Diffraction

7/31/2022 @ 8:30:00 AM - 11:30:00 AM | Salon F
Sponsoring SIG(s): Fiber
Session Chair(s): Rama Madhurapantula; Joseph Orgel; Jesse Hopkins

Abstract Title: **X-ray fiber diffraction to elucidate tissue transition and changes to molecular packing in relation damage**
Presenting Author: **Rama Sashank Madhurapantula, Illinois Institute of Technology**

Abstract Title: **Cardiac myosin filaments are directly regulated by calcium**
Presenting Author: **Weikang Ma**

Abstract Title: **X-ray Fiber Diffraction Reveals Ultrastructural Location and Interactions of the Immunoglobulin Receptor Binding Sequence within Fibrillar Type I Collagen, with Implications for Fibrosis and Autoimmune Conditions.**
Presenting Author: **Joseph Orgel**

Abstract Title: **Small angle x-ray scattering and x-ray diffraction of shark mineralized tissue**
Presenting Author: **Stuart Stock, cell Moelcular biology, Northwestern Univ**

Abstract Title: **MuscleX: Data analysis software for fiber diffraction from muscle and other fibrous protein systems.**
Presenting Author: **Thomas Irving, Biology, Illinois Inst of Technology**

2.1.3 Remote Access

7/31/2022 @ 8:30:00 AM - 11:30:00 AM | Salon E
Sponsoring SIG(s): Light Sources
Session Chair(s): Ana Gonzalez; Uta Ruett

The Covid-19 pandemic and the lockdowns and travel bans enforced over the world have had a big impact in access to large scale experimental facilities, which needed to adapt the way of operation drastically. As a result, many efforts started at various beamlines to develop complex infrastructure for remote experiments. The "Remote Access" session will discuss some of the new protocols, equipment, and also interfaces set up to provide users mail-in or remote services. The impact on the future experimental development and interaction with the users will be examined under various aspects, such as enabling new research approaches by automation or the opportunities for diversity, equity, and inclusion as well as economic justice.

Abstract Title: **Broadening Participation in Structural Biology: New opportunities Enabled by Remote Access**
Presenting Author: **Bill Bauer, Hauptman-Woodward Institute**

Abstract Title: **Next-generation Automation and Remote-access Crystallography**

Presenting Author: **Aina Cohen, Stanford Synchrotron Radiation Lightsource, SLAC, Stanford University**

Abstract Title: **Work-from-Home Synchrotron Science â€“ How we Enabled Remote Operations at NSLS-II**
Presenting Author: **Daniel Olds, Brookhaven National Laboratory**

Abstract Title: **Remote Experiments at SRS Beamlines at Advanced Photon Source**
Presenting Author: **Wenqian Xu**

Abstract Title: **Post-pandemic MX user access at Diamond: blending on-site, remote and fully automated visits**
Presenting Author: **Marco Mazzorana, Diamond Light Source, Ltd. Didcot**

Abstract Title: **Remote access and data collection protocols at AMX and FMX beamlines, BNL, NSLS-II, Upton, NY.**
Presenting Author: **jean jakoncic, BNL**

2.1.4 Macromolecular Structure Under Physiological Conditions

7/31/2022 @ 8:30:00 AM - 11:30:00 AM | Salons G-I
Sponsoring SIG(s): BioMac
Session Chair(s): Leighton Coates; Aina Cohen

Modern protein structures are based nearly exclusively on data collected at cryogenic temperatures. With the cooling process being thought to introduce bias in the functional interpretation of structural results. Structure solution at near physiological conditions can reveal previously hidden structural ensembles in macromolecular structures. Studying room-temperature conformational ensembles using crystallography, NMR, or small angle scattering can reveal motions crucial for catalysis, ligand binding, and allosteric regulation. This session will focus on insights gained from the study of macromolecules at or near physiological conditions.

Abstract Title: **The big thaw: waters freed from cryo-cooling yield dynamic protein-ligand interactions**
Presenting Author: **Timothy Stachowski, St. Jude Children's Research Hospital**

Abstract Title: **New SSRL Remote Access Program Supports Elevated-Temperature and Humidity-Controlled Experiments**
Presenting Author: **Silvia Russi, SSRL Structural Molecular Biology Group, SLAC National Accelerator Laboratory**

Abstract Title: **Towards direct visualization of the reaction coordinates of proteins**
Presenting Author: **Doeke Hekstra, Harvard University**

Abstract Title: **Room-temperature X-ray/neutron crystallography to uncover SARS-CoV-2 main protease function and design potent inhibitors**
Presenting Author: **Andrey Kovalevsky, Oak Ridge National Lab**

Abstract Title: **A robust workflow to study protein correlated motion from ambient temperature crystallography and total scattering**
Presenting Author: **Steve Meisburger, Cornell University**

2.1.5 What I Learned from My First Structures

7/31/2022 @ 8:30:00 AM - 11:30:00 AM | Salons A-B
Sponsoring SIG(s): Service
Session Chair(s): Silvana R. Urcia-Romero; Larry Falvello

This session aims to trace the advance of the methodologies used in structure analysis in terms of the techniques applied by different generations of crystallographers. This will provide a context for the historical development of the technology, techniques, and practices used today. The past high level of technical involvement by the user, and the desire to perfect the results as much as possible have abated, with the advent of automated rapid-throughput analyses accompanied by computer-controlled validation. At the same time, non-routine or previously unfeasible results, involving e.g., twinning, modulation, or ab-initio powder diffraction analysis, can be undertaken today with a reasonable expectation of success. This evolution of techniques and tools has also had a strong impact on the user's educational point of view. It transformed the emphasis 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. Submissions are welcome from all experience levels.

Abstract Title: **Structural insight into the transferrin-iron import system from pathogenic Neisseria**
Presenting Author: **Shubham Dubey, Purdue University**

Abstract Title: **Communication skills learned from my first crystal structures**
Presenting Author: **Louise Dawe, Wilfrid Laurier Univ**

Abstract Title: **The silent art of leveling up: What I learned from my first crystals.**
Presenting Author: **Amy Sarjeant, Bristol-Myers Squibb**

Abstract Title: **Lessons Learned From my First Structures**
Presenting Author: **Brian Toby, Advanced Photon Source 401/B4192, Argonne National Lab**

PL2 Trueblood Award

Airlie McCoy
7/31/2022 @ 1:00:00 PM - 2:00:00 PM | Salon E

Abstract Title: **Molecular Replacement: Past, present and future**
Presenting Author: **Airlie McCoy**

2.2.1 Random Walks in ML: General applications of Machine Learning for Structural Science

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salons G-I
Sponsoring SIG(s): BioMac
Session Chair(s): David Rose; Victoria Drago

Advances in computational power have afforded the expansion of machine learning (ML) into many aspects of research. Complementing sessions on ML in Crystallographic structure solution and CryoEM, this session will provide a forum for other applications of interest to our field, from small molecule and biomacromolecular techniques to automation of routine tasks. Topics (to be confirmed) include crystal screening, RNA structure prediction, small molecule/drug design and others to be identified from submitted abstracts

Abstract Title: **Machine Learning Approaches for Biological Function and Dynamics**
Presenting Author: **Peter Schwander, University Wisconsin-Milwaukee**

Abstract Title: **Advances using machine learning and computational tools for crystal growth and detection**
Presenting Author: **Sarah Bowman, HWI**

Abstract Title: **Accelerating Science with Natural Language Processing in Semantic Scholar**
Presenting Author: **Doug Downey, Allen Institute for AI Seattle, WA**

Abstract Title: **Speeding up Diffraction Analysis using Machine Learning**
Presenting Author: **Hemant Sharma, Argonne National Laboratory**

Abstract Title: **Crystal structure of a fungal polyglycine hydrolase using a RoseTTAFold model**
Presenting Author: **Nicole Fraser, University of Waterloo**

Abstract Title: **Using AlphaFold2 to model TA system protein-protein interactions: A case study with ParDE complexes**
Presenting Author: **Christina Bourne, Chemistry And Biochemistry, Univ Of Oklahoma**

2.2.2 Computer-Aided Materials Design & Development

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salon E
Sponsoring SIG(s): Industrial
Session Chair(s): Susan Reutzel-Edens; Angeles Pulido

Abstract Title: **CheckMyMetal 2.0: a macromolecular metal-binding validation and modeling tool**
Presenting Author: **Michal Gucwa, University of Virginia**

Abstract Title: **Retrospect and Prospect of Small Molecule Microcrystal Electron Diffraction for Pharmaceutical Industry**
Presenting Author: **Darpandeep Aulakh, Bristol Myers Squibb**

Abstract Title: **A Combined Computational and Experimental Study to Understand Solid Form Landscape of beyond Rule of 5 Molecule**
Presenting Author: **Rajni Bhardwaj, Abbvie**

Abstract Title: **Ability of Electron Density Calculation via Three Dimensional Discrete Cosine Transform for Crystallography**
Presenting Author: **Hideo Hiraguchi, The Institution of Professional Engineers, Japan**

Abstract Title: **What Have We Learned From the 7th Blind Test of Crystal Structure Prediction? â€“ Triumphs, Challenges, and Insights**
Presenting Author: **Lily Hunnisett, Cambridge Crystallographic Data Centre**

2.2.3 Structural Science Of Infectious Disease

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salon F
Sponsoring SIG(s): cryo-EM
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Mimi Ho; George Lountos; Daniel Kneller

This session will highlight the application of structural biology to understand host–pathogen interfaces. Examined topics may include, but are not limited to, structural studies on viral, bacterial, and fungal proteins, as well as proteins mediating host-pathogen interactions of eukaryotic and protozoan parasites, with a focus on their functional mechanisms or interactions with host cell metabolites, receptors, and antibodies. Structure-based vaccine design and antibody engineering studies are also welcome. Research aiming to combat infectious diseases by using structural biology methods such as cryo-EM, X-ray crystallography and integrated or complementary techniques will be presented.

Abstract Title: **Cryo-electron tomography of the apicomplexan invasion machinery in its native state reveals rigid body motion of the conoid and docked secretory machinery**
Presenting Author: **Michael Reese, University of Texas, Southwestern Medical Centrer**

Abstract Title: **Bile salt hydrolase substrate preference directs C. difficile infection**
Presenting Author: **Morgan Walker, UNC at Chapel Hill**

Abstract Title: **Mapping of neutralizing monoclonal antibody binding epitopes on Clostridioides difficile toxin proteins**
Presenting Author: **Kevin Huynh**

Abstract Title: **A complex machine for lipid transport across the cell envelope of Mycobacterium tuberculosis**
Presenting Author: **Damian Ekiert, NYU School of Medicine**

Abstract Title: **HIV-1 Rev Regulates Host Transcription and RNA Processing Factor Tat-SF1 to Promote HIV-1 Infectivity**
Presenting Author: **Justin Galardi, University of Rochester Medical Center**

Abstract Title: **Structure-guided coronavirus vaccine design**
Presenting Author: **David Veesler**

2.2.4 The Future Of Past Data For Single xtal, Cryo-EM, Powder & Micro-ED

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salons C-D
Sponsoring SIG(s): Best Practices
Session Chair(s): Lee Daniels; John Rose

Abstract Title: **Evolving the Cambridge Structural Database**
Presenting Author: **Ian Bruno, CCDC Cambridge**

Abstract Title: **RCSB PROTEIN DATA BANK: Enhancing Data Exploration for Future Generations of PDB Users**
Presenting Author: **Stephen Burley, RCSB Protein Data Bank, Rutgers University**

Abstract Title: **80 Years of the Powder Diffraction File™ (PDF®): A Database Perspective**
Presenting Author: **Soorya Kabekkodu, Database, International Ctr For Diff Data New town Square, PA**

Abstract Title: **Getting correlated SAXS data to the outside world with SIMPLE SAXS**
Presenting Author: **Michal Hammel, LBNL**

Abstract Title: **In the Rapidly Advancing Field of MicroED, What Should be Done About Past Data?**
Presenting Author: **Jessica Bruhn, NanoImaging Services**

Abstract Title: **Access to experimental data is the key factor for improvements of scientific reproducibility**
Presenting Author: **Wladek Minor, University of Virginia**

2.2.5 General Interest 2

7/31/2022 @ 2:00:00 PM - 5:00:00 PM | Salons A-B
Sponsoring SIG(s): General Interest
Session Chair(s): Victoria Drago: Alexander Erickson; Elizaveta Katorcha

Abstract Title: **Molecular Structures of Pyridine Derivatives of Some First Row Transition Metal Sulfates**
Presenting Author: **James Golen, UMass Dartmouth**

Abstract Title: **Advanced options of CrysAlis Pro including NoSpher A2 refinement of [Rh2(COOCH3)4]Â·2NCC6H4N(CH3)2**
Presenting Author: **Cassandra Eagle, East Tennessee State University**

Abstract Title: **Development of Orientation Quantification for Single Crystal and Textured Polycrystals from Neutron Transmission Data**
Presenting Author: **Luc Dessieux, ORNL**

Abstract Title: **Approximate Symmetry in Organic Structures in Low-Symmetry Space Groups**
Presenting Author: **Carolyn Brock, University of Kentucky**

Abstract Title: **The effects of CaO/SrO substitution in bioactive glasses: a combined structural and bioactivity study**
Presenting Author: **Margit Fabian, Centre for Energy Research, Environmental Physics**

Abstract Title: **Toward the Molecular Mechanism of a Commercial Ice Nucleating Agent**
Presenting Author: **Jonathan Herrmann, Thermo Fisher Scientific**

Abstract Title: **Powder X-ray Diffraction: direct space, reciprocal space, and between the two**
Presenting Author: **Dubravka Sisak Jung, Dectris Ltd**

Abstract Title: **Next generation MetalJet sources enabling 10µm high brightness high energy beams for High pressure diffraction application**
Presenting Author: **Anasuya Adibhatla, Excillum Inc Grafton, MA**

2.3.1 Would You Publish This

7/31/2022 @ 7:30:00 PM - 9:00:00 PM | Salon F
Sponsoring SIG(s): Service
Session Chair(s): Jeffrey W. Bacon; Matthew L. Brown

When is a structure too poor to publish? How much should scientific impact affect this decision? What are some recommended procedures for publishing poor quality structures? What compromises are involved in the publication of "low quality" structures? If you have ever asked yourself these questions, then share your insights, structures and problems with the small molecule 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, 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.

Abstract Title: **A "Disordered" Gold in a Dicyanoaurate-Lanthanide Coordination Polymer**Presenting Author: **Matthew Brown, University of British Columbia, Okanagan Campus**

Abstract Title: **Can you SQUEEZE an ion? And if not, why not?**
Presenting Author: **William Clegg, Chemistry, School of Natural and Environmental Sciences, Newcastle Univ**

Abstract Title: **Could/Should/Would you publish a modulated metal-coordinated benzothiazole as an unremarkable structure?**
Presenting Author: **Louise Dawe, Wilfrid Laurier Univ**

Abstract Title: **Counterion Quandary**
Presenting Author: **Stacey Smith, Brigham Young University**

Abstract Title: **Evaluating the Quality of MicroED Structures**
Presenting Author: **Jessica Bruhn, NanoImaging Services**

Abstract Title: **HAVE YOU PUBLISHED THIS? Disorder in terminal unsaturated five membered heterocyclic rings**
Presenting Author: **Joseph Reibenspies, Dept of Chemistry, Texas A & M Univ.**

2.3.3 Traversing the APS Dark Period

7/31/2022 @ 7:30:00 PM - 9:00:00 PM | Salon E
Sponsoring SIG(s): Light Sources
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Marian Szebenyi; Bob Fischetti

Abstract Title: **APS-U update and structural biology future directions**
Presenting Author: **Robert Fischetti**

Abstract Title: **Capabilities and capacities of the NSLS-II beamlines, AMX and FMX during the APS upgrade 'dark period'**

Presenting Author: **jean jakoncic, BNL**

Abstract Title: **MacCHESS: MX and BioSAXS capabilities**
Presenting Author: **Doletha Szebenyi, MacCHESS, Cornell Univ Ithaca, NY**

Abstract Title: **Macromolecular crystallography facilities at MAX IV**
Presenting Author: **Ana Gonzalez, MAX IV Lund**

Abstract Title: **The Structural Molecular Biology Program at the Stanford Synchrotron Radiation Lightsource**
Presenting Author: **Aina Cohen, Stanford Synchrotron Radiation Lightsource, SLAC, Stanford University**

PS2 POSTER SESSION 2

7/31/2022 @ 5:30:00 PM - 7:30:00 PM
Exhibit Hall

Abstract Title: **Cryo-EM SPA for Structural Understanding of A-to-I RNA Editing: Human Adenosine Deaminase Acting on RNA 2 (ADAR2) Complexed with dsRNA**
Presenting Author: **Melissa Matthews, Okinawa Institute of Science and Technology**

Abstract Title: **Crystal Structures of Polymerized LiCl and dimethyl sulfoxide in the form of {2LiClâ€¢3DMSO}âˆž and {LiClâ€¢DMSO}âˆž**
Presenting Author: **Nichole Valdez, Sandia National Laboratories**

Abstract Title: **Detailed mechanism of catalysis by tetrameric L-glutaminase-asparaginase from Pseudomonas 7A (PGA)**
Presenting Author: **Pawel Strzelczyk, Center for Structural Biology, Center for Cancer Research, National Cancer Institute**

Abstract Title: **Development of Novel Chemical Probes for the Treatment of Lyme Disease**
Presenting Author: **Mark Kowalewski, UNC Chapel Hill**

Abstract Title: **Development update of PIONEER, a single-crystal neutron diffractometer at the Second Target Station, ORNL**
Presenting Author: **Yaohua Liu, Oak Ridge National Laboratory**

Abstract Title: **Glu445Ala in DesD Crystallization and ATP/AMP binding with Kinetics**

Presenting Author: **Pablo Paredes**

Abstract Title: **Investigation of a Putative Polysaccharide Deacetylase from Gut Microbe [i]Bacteroides ovatus[/i]**
Presenting Author: **Krystle McLaughlin, Vassar College**

Abstract Title: **New and Updated Phenix features**
Presenting Author: **Billy Poon, Lawrence Berkeley National Laboratory**

Abstract Title: **Predicting Target Binding Sites in Plant Immune Receptors**
Presenting Author: **Daniil Prigozhin, Lawrence Berkeley National Laboratory**

Abstract Title: **Structural insight on ubiquitination of NEMO for canonical activation of NF-ÐºB**
Presenting Author: **Mamta Iyer, Chapman University**

Abstract Title: **Structural Studies of TDE0362: A Virulence Factor in [i] Treponema denticola [/i]**
Presenting Author: **Nicholas Clark, Department of Structural Biology, State University of New York: University at Buffalo**

Abstract Title: **Structures of MfnG, an O-methyltranseferase involved in the biosynthese of marformycins, from multiple crystal forms**
Presenting Author: **Mitchell D. Miller, Rice University**

Abstract Title: **Study of L-captopril Binding to VIM-20 by X-ray Crystallography Method**
Presenting Author: **Surendra Silwal, Miami University**

Abstract Title: **The Role of Glu467 in NIS Synthetase DesD: Structure, Thermodynamics, and Kinetics.**
Presenting Author: **Ashley Dumas, California Lutheran University**

Abstract Title: **Towards understanding the conformational changes behind electron bifurcation in thermophilic metalloenzymes using small-angle X-ray scattering**
Presenting Author: **Dan Murray, Lawrence Berkeley National Laboratory**

Abstract Title: **Understanding the role of pyridoxal reductase (PDXI) in pyridoxal 5â€™-phosphate (PLP) homeostasis.**
Presenting Author: **Akua Donkor, Virginia Commonwealth University**

Abstract Title: **Viral RNA Dependent RNA Polymerase forms Amyloids Like Fibrils via Liquid-Liquid Phase Separation**
Presenting Author: **Soni Kaundal, Baylor College of Medicine, Houston**

Abstract Title: **X-ray Crystallographic Studies of pri-miR-21**
Presenting Author: **Doug Davies, UCB**

Abstract Title: **Features in selected area continuous rotation electron diffraction measurements that may be sensitive to molecular handedness of 3D crystals**
Presenting Author: **Niko Vlahakis, University of California, Los Angeles**

Abstract Title: **Atomic Structure Transformations of C-Doped Ge2Sb2Te5 Using In-Situ X-Ray Scattering**
Presenting Author: **John Langhout, University of Florida**

Abstract Title: **Effect of TELSAM-Target Protein Linkers on Crystal Formation and Quality**
Presenting Author: **Celeste Litchfield, Brigham Young University**

Abstract Title: **Synthesis and Characterization of Sr[sub]12[/sub]Al[sub]14[/sub]O[sub]33[/sub]**
Presenting Author: **Claudia Rawn, University of Tennessee, Knoxville**

Abstract Title: **Leveraging Quantum-Chemical [i]In Silico[/i] Techniques To Determine Guest Binding Energies for the Crystalline Sponge Method**
Presenting Author: **Timothy Ramadhar, Howard University**

Abstract Title: **Progress towards Increasing Automation and Sample Capacity at the GM/CA Beamlines for the upgraded APS (APS-U)**
Presenting Author: **Craig Ogata, Argonne National Lab**

Abstract Title: **Unnecessarily Complicated Research**
Presenting Author: **Larry Andrews, Ronin Institute**

Monday, August 1, 2022

3.1.1 Frontiers Of Local Structure Analysis: Total Scattering, Single-Crystal Diffuse Scattering & More

8/1/2022 @ 8:30:00 AM - 11:30:00 AM | Salons A-B
Sponsoring SIG(s): Neutrons/Materials/Powder
Session Chair(s): Huiwen Ji; Matthew Krogstad

As our ability to investigate and understand crystal structures has improved, we have increasingly seen the importance of locally-correlated structures within well-ordered materials. Observing local structure via pair distribution function (PDF) measurement in powders or with single crystal diffuse scattering has become increasingly accessible, with improvements in both instrumentation and computing allowing for more comprehensive and detailed measurements and more complete and better-guided analysis. In this session, we will show examples of powder-based PDF studies and single crystal diffuse scattering and how each can help determine local structures within crystalline materials and reveal structure-property relationships that were previously overlooked. Contributions on the aforementioned two topics from both X-ray and neutron areas are welcome.

Abstract Title: **New Developments in the Use of Single Crystal Diffuse Scattering to Probe Nanoscale Correlations in Crystalline Materials**
Presenting Author: **Stephan Rosenkranz, Argonne National Laboratory**

Abstract Title: **Integrated analysis for both diffuse and Bragg single crystal neutron scattering**
Presenting Author: **Zachary Morgan, Oak Ridge National Laboratory**

Abstract Title: **Epitaxial intergrowths and local oxide displacements in natural bixbyite**
Presenting Author: **Kristoffer Støckler, Aarhus University Aarhus C**

Abstract Title: **Recent Advances in Magnetic PDF Analysis: A Case Study with MnTe**
Presenting Author: **Benjamin Frandsen, Brigham Young University**

Abstract Title: **New development for neutron total scattering data reduction and analysis**
Presenting Author: **Yuanpeng Zhang, ORNL**

Abstract Title: **Structural analysis of novel materials via grazing-incidence high-energy total X-ray scattering**

Presenting Author: **Olaf Borkiewicz, X-Ray Science Division, Argonne National Laboratory**

3.1.2 Home-Built Software & Hardware

8/1/2022 @ 8:30:00 AM - 11:30:00 AM | Salons C-D
Sponsoring SIG(s): Service
Session Chair(s): Victor Young; Larry Falvello

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

Abstract Title: **HP-MX at MacCHESS: High pressure macromolecular crystallography in a DAC**
Presenting Author: **Doletha Szebenyi, MacCHESS, Cornell Univ Ithaca, NY**

Abstract Title: **New algorithms for interpreting time-resolved SAXS data**
Presenting Author: **Stephen Moore, University at Buffalo Buffalo, NY**

Abstract Title: **XtremeD: A new single crystal and powder diffractometer designed for measurements at extreme conditions of pressure and magnetic fields**
Presenting Author: **Stephen Moore, University at Buffalo Buffalo, NY**

Abstract Title: **Easing script writing on Google Colab with structural biology snippets**
Presenting Author: **Blaine Mooers, Universtiy of Oklahoma Health Sciences Center**

Abstract Title: **Software tools for neutron wavelength-resolved Laue diffraction in multi-dimensional diffraction and parameter spaces**
Presenting Author: **Xiaoping Wang, Neutron Scattering Division, Oak Ridge National Laboratory**

Abstract Title: **What can be done after APS-upgrade at NSF's ChemMatCARS Advanced Crystallography Program?**
Presenting Author: **Yu-Sheng Chen, University of Chicago Limont, IL**

3.1.3 Structure and Regulation of Protein-Nucleic Acid Complexes

8/1/2022 @ 8:30:00 AM - 11:30:00 AM | Salon F
Sponsoring SIG(s): BioMac
Session Chair(s): Jason Stagno; Clara Kielkopf

Protein-nucleic acid complexes regulate gene expression in hosts and pathogens. The 3D structural underpinnings of these key macromolecular machines are critical for understanding gene regulation by numerous pathways and to define potential pharmaceutical targets. This session will present cutting-edge research on protein-RNA and protein-DNA structures, with emphasis on noncoding RNAs, post-transcriptional modifications, and new insights from cryo-electron microscopy.

Abstract Title: **Sleeping Beauty Redux â€“ Resting Ribosomes in Neurons**
Presenting Author: **Sarah Loerch, University of California, Santa C**

Abstract Title: **Structural basis of Cas1-2/3 integrase recruitment to the CRISPR leader-repeat boundary**
Presenting Author: **Andrew Santiago-Frangos, Montana State Unversity**

Abstract Title: **Discovery of a bacterial riboswitch class that binds metabolites in a stacked configuration for cooperative gene regulation**
Presenting Author: **Joseph Wedekind, Dept of Biochemistry & Biophysics, University of Rochester**

Abstract Title: **Structural basis for host tRNA control of HIV-1 Gag localization**
Presenting Author: **Charles Bou-Nader, National Institute of Diabetes and Digestive and Kidney Diseases - NIH**

Abstract Title: **Structural Basis for RNA editing by ADARs**
Presenting Author: **Andrew Fisher, Depts of Chemistry & Mol Cell Bio, Univ of California Davis**

Abstract Title: **Exploring ATAD2 bromodomain structure and function differences in the dynamic epigenetic landscape**
Presenting Author: **Kiera Malone, University of Vermont**

Abstract Title: **Cryo-EM reveals conformational dynamics in a multifunctional viral RNA**
Presenting Author: **Jeffrey Kieft, University of Colorado Anschutz Medical Campus, School fo Medicine**

3.1.4 Open Exchanges In Crystallographic Education

8/1/2022 @ 8:30:00 AM - 11:30:00 AM | Salon E
Sponsoring SIG(s): General Interest
Session Chair(s): Kraig Wheeler: Yinka Olatunji-Ojo

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: **Online and 3D-printed resources for introducing crystallographic concepts**
Presenting Author: **Dean Johnston, Chemistry, Otterbein Univ**

Abstract Title: **Partial Charge Determination of SC-XRD Data with Refinement of Occupancy of Spherical Atoms (ROSA)**
Presenting Author: **Taylor Keller, Temple University**

Abstract Title: **Using Protein Crystallography to engage HBCU students in biochemistry**
Presenting Author: **Oluwatoyin Asojo, Hampton University**

Abstract Title: **Addressing Misconceptions in Chemical Crystallography**
Presenting Author: **Shao-Liang Zheng, Harvard University**

Abstract Title: **ACA Crystallographic Literacy: A Web Portal for all Things Crystallographic, by Crystallographers.**
Presenting Author: **Allen Oliver, Dept of Chemistry & Biochemistry, Univ of Notre Dame**

Abstract Title: **Approaches to structural chemistry education at the Cambridge Crystallographic Data Centre**
Presenting Author: **Yinka Olatunji-Ojo, The Cambridge Crystallographic Data Centre**

Abstract Title: **Exploring Molecular Structure with Symmetry, Chirality and Shape Measures**
Presenting Author: **Inbal Tuvi-Arad, The Open University of Israel**

Abstract Title: **Structures vs articles? Teaching students the place of primary crystal structure databases in the information landscape**
Presenting Author: **Judith Currano, University of Pennsylvania**

Abstract Title: **Teaching crystallography for all**
Presenting Author: **Natalia Alvarez, Facultad de Quimica, UdelaR**

3.1.5 Scanning Imaging & Tomography Based on Scattering Contrast

8/1/2022 @ 8:30:00 AM - 11:30:00 AM | Salons G-I
Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Lin Yang; Masa Fukuto

In scattering measurements on complex structures such as biological tissues and fabricated devices, all structural components within the illuminated volume contribute to the observed scattering intensity. With a small x-ray beam as the probe, raster scanning can be used as an imaging technique to map out the distribution of these structural components. Tomographic data collection is also possible to resolve structural distributions in 3D. This session is intended to inform the community of the current research examples, in hope of inspiring wider application and further development (e.g. the use of computation and machine learning to distinguish different structural components) of this technique.

Abstract Title: **Scanning x-ray microdiffraction mapping of fibrillar polymorphs in Alzheimer's disease**
Presenting Author: **Lee Makowski, Northeastern University Boston, MA**

Abstract Title: **Scanning the brain using X-ray scattering**
Presenting Author: **Marios Georgiadis, Stanford University School of Medicine**

Abstract Title: **Structural Reconstruction of Organic Semiconductor Thin Films via Grazing-Incidence Diffraction Tomography**
Presenting Author: **Ruipeng Li, Brookhaven national lab**

Abstract Title: **X-ray Ptychography and SAXS imaging of nanoparticle assemblies on substrates**
Presenting Author: **Byeongdu Lee, Argonne National Laboratory**

Abstract Title: **Study the hierarchical structure of materials by scanning Micro/Nano diffraction**
Presenting Author: **jiliang liu, ESRF**

Abstract Title: **Scanning Mapping and Tomographic Imaging of Cellulose in Plant Tissues**
Presenting Author: **Lin Yang, Brookhaven National Laboratory**

PL3 Bau Neutron Diffraction Award

Arthur J. Schultz
8/1/2022 @ 1:00:00 PM - 2:00:00 PM | Salon E

Abstract Title: **Single-Crystal Time-of-Flight Neutron Diffraction: IPNS to SNS**
Presenting Author: **Arthur Schultz, X-Ray Science Division, Argonne National Lab**

3.2.1 Educating The New Generation Of Users

8/1/2022 @ 2:00:00 PM - 5:00:00 PM | Salons A-B
Sponsoring SIG(s): Light Sources
Co-Sponsoring SIG(s):
Session Chair(s): Clyde Smith; Eddie Snell

Many facilities run courses to educate the next generation of users and pass on tips, tricks, and new developments. These span a wide range of areas and techniques. From a source perspective, they include synchrotron, neutron, and cryo-EM facilities. From a technical perspective, there are courses that focus on whole areas of structural biology and specific techniques. In this session, we invite organizers of these courses to describe best practices for educating the community, and the impact they are making on the next generation of users. We encourage a snapshot of the training to be provided and aim to serve as a forum to advertise these workshops and courses, publicizing them to the community.

Abstract Title: **The National High-Throughput Crystallization Center and coming hands-on workshops**
Presenting Author: **Sarah Bowman, HWI**

Abstract Title: **RapiData at SSRL - Data Collection and Structure Solving: A Practical Course in Macromolecular X-Ray Diffraction Measurement**
Presenting Author: **Silvia Russi, SSRL Structural Molecular Biology Group, SLAC National Accelerator Laboratory**

Abstract Title: **"Workbenches": Means to prepare the future light source research community?**
Presenting Author: **Vivian Stojanoff**

Abstract Title: **"Enabling access to cryoEM technologies by novice practitioners through access and training at multiple scales**
Presenting Author: **Christina Zimanyi, New York Structural Biology Center**

Abstract Title: **Teaching Small Angle X-ray Scattering for Structural Biology**
Presenting Author: **Thomas Weiss, Stanford University / SLAC**

3.2.2 Fragment Based Drug Discovery

8/1/2022 @ 2:00:00 PM - 5:00:00 PM | Salons C-D
Sponsoring SIG(s): Industrial
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Matt Clifton; John Tanner

Fragment Based Drug Discovery (FBDD) utilizes small molecule compounds to help identify starting points in the drug discovery process. This process allowed for the discovery of lead compounds for difficult protein targets with small/shallow pockets or protein-protein interactions. In contrast to other screening techniques such as High-Throughput Screening (HTS) or DNA-encoded Libraries (DEL), FBDD utilizes small libraries of molecules (< 2000) with molecular weights less than ~200 Da. FBDD has been key in the development of multiple approved drugs and dozens of other drugs in clinical trials. This session will focus on the biophysical and structural techniques used in FBDD to identify initial starting points, optimization by fragment growing/linking, and the route to lead optimization.

Abstract Title: **Structure-based design of MRTX1719: an MTA-cooperative PRMT5 Inhibitor for treatment of MTAP-deleted cancers**
Presenting Author: **Robin Gunn, Mirati Therapeutics**

Abstract Title: **Fragment-Screening by Crystallography at the Helmholtz-Zentrum Berlin â€“ workflow, tools and procedures**
Presenting Author: **Manfred Weiss, Macromolecular Crystallography, Helmholtz-Zentrum Berlin**

Abstract Title: **Protein engineering enables a fragment-based drug design platform to inhibit the anti-apoptotic protein MCL1**
Presenting Author: **Matt Clifton**

Abstract Title: **Structure-guided development of small molecule modulators of nuclear receptor LRH-1**
Presenting Author: **Michael Cato, Emory University Decatur, GA**

Abstract Title: **Exposing the DRome ("DNA Repair-ome")**
Presenting Author: **Debanu Das, Accelero Biostructures**

3.2.3 Time-resolved Structural Dynamics and Kinetic Processes

8/1/2022 @ 2:00:00 PM - 5:00:00 PM | Salon E
Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Tom Grant; Venky Pingali; Wellington Leite

Structural biology to date has mostly been described using static snapshots of macromolecules. Recent developments in new sources, sample preparation techniques, and software developments have enabled researchers to probe time-resolved structural dynamics of macromolecules from the ultrafast femtosecond time-scales up to milliseconds or longer. These developments allow chemically and functionally biological intermediates to be studied with unprecedented spatial and temporal resolution. Similarly, there have been developments that allow probing components within complex systems undergoing structural changes during biochemical and biotechnological processes. This session aims to cover the latest developments in the field of time-resolved structural dynamics and kinetic processes from a variety of techniques using X-ray, neutron, or electron sources in solution or in crystals.

Abstract Title: **Revealing the structural dynamics of biomolecules with x-rays and XFELs**
Presenting Author: **Lois Pollack, Cornell University**

Abstract Title: **Using time-resolved scattering techniques to study nanoscale wood-water interactions**
Presenting Author: **Nayomi Plaza, Forest Service Forest Products Laboratory**

Abstract Title: **In Crystallo Observation of Three Metal Ion Promoted DNA Polymerase Misincorporation**
Presenting Author: **Caleb Chang, Rice University**

Abstract Title: **Chaotic Advection Mixer for Capturing Transient States of Diverse Biological Macromolecular Systems with Time-Resolved Small Angle X-ray Scattering**
Presenting Author: **Kara Zielinski, Cornell University**

Abstract Title: **Time-Resolved Î²-lactam Cleavage by L1 Metallo-Î²-Lactamase**
Presenting Author: **Andrzej Joachimiak, Argonne National Laboratory/University of Chicago**

Abstract Title: **Protein structural dynamics revealed by time-resolved x-ray liquidography**
Presenting Author: **Hyotcherl Ihee, Dept of Chemistry, KAIST, & Inst for Basic Science Daejeon**

3.2.4 Opening the Black Box

8/1/2022 @ 2:00:00 PM - 5:00:00 PM | Salon F
Sponsoring SIG(s): Small Molecule
Session Chair(s): Bill Clegg; Carla Slebodnick

A push-button automation approach to crystal structure determination by X-ray diffraction is all very well for the vendors and for inexperienced users, but a practicing crystallographer is likely to encounter samples requiring a better grasp of the underlying theory, instrumentation, and software to understand what's happening, to interpret the results sensibly, and to know what to do when the automatic methods don't deliver the goods. In this session we seek to prise open some of the popular 'black boxes' and reveal what's inside, so that an informed user has some idea how to tinker around with the controls and maybe even rewire some of the inner workings. We hope to have access to insider knowledge about procedures such as the automatic derivation of unit cells from initial diffraction images, the choice of space groups, how structures are determined by charge flipping and dual-space approaches, and how constraints, restraints and other refinement tricks and tools work.

Abstract Title: **How do initial diffraction images get turned into a unit cell and what can I do when it doesn't work?**
Presenting Author: **William Clegg, Chemistry, School of Natural and Environmental Sciences, Newcastle Univ**

Abstract Title: **A survey of applied corrections to measured Bragg and diffuse diffraction intensities for meaningful structure factor amplitudes**
Presenting Author: **Christina Hoffmann**

Abstract Title: **Forensic Crystallography - or how to improve your stubborn refinement**
Presenting Author: **Anthony Linden, Department of Chemistry, University of Zurich**

Abstract Title: **Dual-space methods: a modern take on overcoming the phase problem!**
Presenting Author: **Allen Oliver, Dept of Chemistry & Biochemistry, Univ of Notre Dame**

Abstract Title: **Making the Most out of Non-Ideal Samples: When and How to Use Problem Datasets**
Presenting Author: **Steven Kelley, University of Missouri Columbia**

3.2.5 Hot Structures

8/1/2022 @ 2:00:00 PM - 5:00:00 PM | Salon G-I
Sponsoring SIG(s): cryo-EM
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Melody Campbell; Samantha Powell

This session will be comprised of talks describing exciting new macromolecular structures. Talks focusing on structures will be highlighted from across all disciplines of structural biology (Cryo-EM, X-ray Crystallography, NMR, SAXS, etc.). The majority of the talks will be selected from submitted abstracts

Abstract Title: **Structural and Bioinformatic Analysis of an Ancient Enzyme Family**
Presenting Author: **Audrey Burnim, Cornell University**

Abstract Title: **Structures and mechanism of a type IIS restriction endonuclease: PaqCI**
Presenting Author: **Madison Kennedy, University of Washington**

Abstract Title: **Structure of a HIV-1 IN-Allosteric Inhibitor Complex at 2.93 Å Resolution: Routes to Inhibitor Optimization**
Presenting Author: **Kushol Gupta, Biochemistry & Biophysics, Univ of Pennsylvania**

Abstract Title: **Activated dioxygen intermediates at the copper-active site of a lytic polysaccharide monooxygenase**

Presenting Author: **Flora Meilleur**

Abstract Title: **CryoEM structure of a multivalent ubiquitin ligase complex**
Presenting Author: **Gilbert Privé, Princess Margaret Cancer Centre, Univ Health Network Toronto**

PS3 POSTER SESSION 3

8/1/2022 @ 5:30:00 PM - 7:30:00 PM
Exhibit Hall

Abstract Title: **A drug and ATP binding site in type 1 ryanodine receptor**
Presenting Author: **Zephan Melville, Columbia University Irving Medical Center**

Abstract Title: **A molecular view of stress relief in Bartonella Quintana: Crystal structures PhyR, PhyR complexed with NepR, and RpoE complexed with NepR**
Presenting Author: **David Dranow, UCB / SSGCID**

Abstract Title: **Allosteric activation of choanoflagellate soluble guanylate cyclase and the evolution of NO signaling in animals**
Presenting Author: **William Thomas, UC Berkeley**

Abstract Title: **Capsid structure of a densovirus causing mass mortality in larval darkling beetles (Zophobas morio)**
Presenting Author: **Judit Penzes, Rutgers University**

Abstract Title: **DESIGN AND CHARACTERIZATION OF CIRCULARLY PERMUTED CASPASE-2 MUTANTS AND THEIR USE IN EVALUATION OF NOVEL CASPASE-2 INHIBITORS**
Presenting Author: **Jessica Fuller, University of Minnesota**

Abstract Title: **Modelling and refinement of hydrogen atoms: new developments in REFMAC5**
Presenting Author: **Lucrezia Catapano, King's College London/ MRC Laboratory of Molecular Biology**

Abstract Title: **Probing ligand-binding of endothiapepsin by â€œtemperature-resolvedâ€� macromolecular crystallography**
Presenting Author: **Chia-Ying Huang, Swiss Light Source/PSI**

Abstract Title: **Structural Insights Into A Novel Collapsed Confirmation of Human ABCB1 In A Lipid Environment**
Presenting Author: **Devanshu Kurre, Hormel Institute/University of Minnesota**

Abstract Title: **Structures of Antibodies and Nanobodies in Complex with Spike/RBD: The vital role of CDR loops in capturing epitopes**
Presenting Author: **Christopher T Boughter, Computational Biology Section, LISB/NIAID/NIH**

Abstract Title: **The Ensemble of TELSAM Crystallization Behaviors**
Presenting Author: **Maria Pedroza, Brigham Young University**

Abstract Title: **Reaction of Monosaccharides with Substituted Anilines and Phenylhydrazines: Schiff Bases vs. Glycosylamines as Crystalline Products**
Presenting Author: **William Ojala, Chemistry, University of St Thomas**

Abstract Title: **Stimulation of mitochondrial Endonuclease G by natural polyphenols to degrade damaged DNA**
Presenting Author: **Hanna Yuan, Academia Sinica, Institute of Molecular Biology**

Abstract Title: **Structural Studies of DNMT1-DNA Complexes with a Reversible Series of Dicyanopyridine Containing Selective, Non-Nucleoside Inhibitors**
Presenting Author: **John Horton, MD Anderson Cancer Center of The University of Texas**

Abstract Title: **Structural delineation of malaria vaccine antigen Pfs230D1 binding to a potent transmission reducing human antibody**
Presenting Author: **Wai Kwan Tang**

Abstract Title: **Structural Characterization and Mechanistic Insights into Pathogenic Fungal Acetyl-CoA Synthetases**
Presenting Author: **Nicholas DeBouver, UCB Biosciences**

Abstract Title: **Evaluating crystal structures of LpxC from Pseudomonas aeruginosa (paLpxC) in complex with new small molecule inhibitors**
Presenting Author: **Silvia Delker, UCB**

Abstract Title: **The Effect of Holliday Junction Sequence and Isomeric Form on the Self-assembly of Rationally Designed DNA Crystals**
Presenting Author: **Chad Simmons, Arizona State University**

Abstract Title: **Gentle Equilibration of Macromolecular Crystals to New Solutions with Minimal Handling**
Presenting Author: **Douglas Juers**

Abstract Title: **Protein-Binding Proteins Designed from Target Structural Information**
Presenting Author: **Nicholas DeBouver,**

Abstract Title: **Synthesis, characterization and [i]in vitro[/i] antitumor screening of novel gold (I) & (III) complexes**
Presenting Author: **Joe Tanski, Vassar College**

Abstract Title: **Supramolecular structuring of cyclo-dipeptides**
Presenting Author: **Joanna Bojarska, Technical University**

Abstract Title: **Repositioning Small-Molecule Crystallography to Educate Next Generation of Users**
Presenting Author: **Shao-Liang Zheng, Harvard University**

Abstract Title: **Mechanochemical synthesis, crystal structure analysis and solid-state characterization of quininium aspirinate, a drug-drug salt**
Presenting Author: **SILVINA PAGOLA, Old Dominion University, Department of Chemistry & Biochemistry**

Abstract Title: **The unified (UNI) system of magnetic space-group symbols**
Presenting Author: **Branton Campbell, Brigham Young University**

Abstract Title: **Screening approaches that explore chemical space in order to identify suitable starting conditions for structure determination by cryoEM or other methods**
Presenting Author: **Patrick Shaw Stewart, Douglas Instruments Ltd**

Abstract Title: **The Berkeley Center for Structural Biology: A suite of macromolecular crystallography beamlines at the Advanced Light Source**
Presenting Author: **Daniil Prigozhin, Lawrence Berkeley National Laboratory**

Abstract Title: **The National Center for CryoEM Access and Training: Utilizing CryoEM Merit Badges to Accelerate Access to CryoEM Technology**
Presenting Author: **Edward Eng, New York Structural Biology Center**

Abstract Title: **CryoEM analysis workflow for viral vector-based gene therapy and vaccine development**
Presenting Author: **Timothy Wilson, NanoImaging Services**

Abstract Title: **Bound! New Protein-Drug Matching Card Game from the CCDC and PDB-101**
Presenting Author: **Ilaria Gimondi, The Cambridge Crystallographic Data Centre**

4.1.1 Materials For Our Future: Structural Insights Into Energy Materials And Sustainable Materials

8/2/2022 @ 8:30:00 AM - 11:30:00 AM | Salon F
Sponsoring SIG(s): Neutrons/Materials/Powder
Session Chair(s): Joya Cooley; Michelle Dolgos

Abstract Title: **Examination of local distortions and long-range polarity in pyrochlore oxides through total scattering techniques**
Presenting Author: **Geneva Laurita, Bates College**

Abstract Title: **Structural insight into hydrogen isotope separation mechanism in a ultramicroporous material**
Presenting Author: **Cheng Li, Oak Ridge National Laboratory**

Abstract Title: **Neutron and X-ray Scattering to Characterize Adsorbents and Their Hosts**
Presenting Author: **Craig Brown, NIST**

Abstract Title: **Infiltration of Single-Ion Magnets into Metal-Organic Frameworks for Controlled Nanostructuration: Translation of Density Functional Theory to the Experiment**
Presenting Author: **Monu Joy, Clarkson University**

Abstract Title: **Structural insights into Li-based energy storage by metastable niobates**
Presenting Author: **Megan Butala, University of Florida**

Abstract Title: **High brightness MetalJet x-ray source for MOFs/COFs structure determinations**
Presenting Author: **Julius Hållstedt, Excillum Solna**

4.1.2 Hardware And Software Standardization In Structural Biology

8/2/2022 @ 8:30:00 AM - 11:30:00 AM | Salons A-B
Sponsoring SIG(s): Best Pract./Light Sources
Session Chair(s): Martin Fuchs; Raquel Bromberg

This session is dedicated to the memory of Andreas Förster.

Structural biology researchers now access light sources and electron microscope facilities almost exclusively from remote locations due to the pandemic. This is expected to continue in the future. As a result, more users are exposed to different facilities and their varied interfaces and methods. The upcoming APS shutdown will further increase crystallographers' mobility in the US.

In electron microscopy the field is rapidly evolving, and in crystallography, new and renewed crystallographic methods like serial crystallography, room temperature data-collection, and machine learning further contribute to a variable synchrotron environment. This is a great time for finding standards and collaboration opportunities, to improve the users' experience and scientific output, and best use staff and facility resources.

From the wetlab, over beamlines and microscopes, to data processing and depositing final results, this is a wide field. We invite contributions from facilities, academia and industry that provide an overview of standardization possibilities in the different areas, with the speakers not talking exclusively about their own work. This session aims to foster collaboration between facilities and to discuss new standards and compatibility between existing solutions - with the goal to allow researchers to collect better data and focus on their science rather than technicalities.

Abstract Title: **Enabling high-energy, large-unit-cell, ultra-high-resolution X-ray crystallography on beamline P14@PETRAIII**
Presenting Author: **Clemens Schulze-Briese, DECTRIS Ltd.**

Abstract Title: **Introduction to Hardware And Software Standardization In Macromolecular Crystallography**
Presenting Author: **Martin Fuchs, Photon Sciences, Brookhaven National Lab**

Abstract Title: **Standardization in MX as a collaborative tool for the success of the structural biology user communities**
Presenting Author: **Daniele de Sanctis, ESRF**

Abstract Title: **Industrial MX User – Standardized Software / Hardware**
Presenting Author: **Joshua Carter, Helix BioStructures, LLC**

Abstract Title: **Metadata standards in x-ray crystallography**
Presenting Author: **Aaron Brewster, Lawrence Berkeley National Lab**

Abstract Title: **Improving the quality of 3D cryo-EM structure data at the Worldwide Protein Data Bank**
Presenting Author: **Justin Flatt**

Abstract Title: **The conundrum of depositing half-maps for experimental cryoEM data**
Presenting Author: **Zbyszek Otwinowski, UT Southwestern**

Abstract Title: **cryoHub: A customizable web interface for cryo-EM data processing**
Presenting Author: **Yilai Li, University of Michigan**

4.1.3 Frontiers in SAS

8/2/2022 @ 8:30:00 AM - 11:30:00 AM | Salons C-D
Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Jesse Hopkins; Max Watkins

Recent advances in light sources, experimental methods and computational algorithms have enabled exciting new discoveries using small angle scattering (SAS). This session is devoted to discussing the latest advances in methods and applications of X-ray and neutron SAS. The primary aim is to bring together cutting-edge advances utilizing SAS on both soft matter and biological systems, including time-resolved studies, contrast matching, dynamic and flexible systems, hybrid modeling, novel experimental apparatus and methods, and new computational approaches. This session will reflect the state of the art in SAS methods.

Abstract Title: **Intradomain interactions in c-SRC revealed by domain specific deuteration and small-angle neutron scattering**
Presenting Author: **Viswanathan Gurumoorthy,**

Abstract Title: **Understanding Self Assembly Under Reservoir Like Conditions**
Presenting Author: **Thomas Fitzgibbons, Analytical Sciences, The DOW Chemical Company**

Abstract Title: **Beyond microns - next generation USAXS instrument at upgraded APS**
Presenting Author: **Jan Ilavsky**

Abstract Title: **A multi-step nucleation process determines the kinetics of prion-like domain phase separation**

Presenting Author: **Erik Martin, Dewpoint Therapeutics**

Abstract Title: **Assembly of deuterated phospholipid nanodiscs for Small-Angle Neutron Scattering studies**
Presenting Author: **Wellington Leite, Oak Ridge National Laboratory**

Abstract Title: **Remote Experiments and Automation for biological SAXS at SSRL BL4-2**
Presenting Author: **Thomas Weiss, Stanford University / SLAC**

Abstract Title: **Structural changes of oxygen-sensing transcription factor revealed through anoxic small-angle X-ray scattering**
Presenting Author: **Gabrielle Illava, Cornell**

4.1.4 Remembering Carroll K. Johnson: Structure Visualization from ORTEP to the Future

8/2/2022 @ 8:30:00 AM - 11:30:00 AM | Salon E
Sponsoring SIG(s): Service/BioMac
Session Chair(s): Nichole R. Valdez; David Goodsell

Chemical structure, whether it be molecular or crystallographic, is an inherently three-dimensional property that is most often displayed on two-dimensional surfaces, such as printed images or computer screens. Advancements in visualization technology have created new ways for scientists to present dynamic processes and structural data in engaging and helpful formats. This session focuses on communicating science through visualization using the latest developments in 2D and 3D methods. This includes, but is not limited to, animation and rendering techniques, lighting and coloring effects, VR, AR, and 3D printing, and other advanced display methods used by structural scientists to visualize molecular interactions, reactions, protein structures, crystal structures, and crystallography principles, or to aid in structure-based drug design.

Abstract Title: **Perceptualizing our Molecular World**
Presenting Author: **Arthur Olson, Scripps Research**

Abstract Title: **Immersive structure exploration with Virtual Reality**
Presenting Author: **Martina Maritan, Nanome inc**

Abstract Title: **The Old and the New - Complementary uses of CPK and 3D Printed Atom Models**

Presenting Author: **Dale Tronrud**

Abstract Title: **Blender, a Free Tool to Import Data from All Fields of Crystallography and Export to the Virtual and Physical Space**
Presenting Author: **Michael Aristov, Chemistry, UW Madison**

4.1.5 Cool Structures I

8/2/2022 @ 8:30:00 AM - 11:30:00 AM | Salons G-I
Sponsoring SIG(s): Small Molecule
Session Chair(s): Diane Dickie; Dan Decato

Structure elucidation from nanometer-sized crystals has positioned microcrystal electron diffraction at the forefront of structural science. This session will feature small molecule (< 150 atoms per molecule) structures solved using MicroED and aims to highlight successes made possible by MicroED. Speakers will be selected from contributed abstracts. Submissions from students are encouraged.

Abstract Title: **Departures from Near Inversion Symmetry Using Amino Acid Hydrogen Oxalate Quasiracemates**
Presenting Author: **Kraig Wheeler, Dept of Chemistry, Whitworth University**

Abstract Title: **Preparation of Metal Based Quasiracemates: Copper(II) Complexes of Substituted N-Phthaloylalaninato and N-Benzoylalanninato Ligands**
Presenting Author: **Mark Whitener, Chemistry & Biochemistry, Montclair State Univ Upper Montclair, NJ**

Abstract Title: **Two Jahn-Teller systems involved in different kinds of crystal-to-crystal transformations**
Presenting Author: **Larry Falvello, Dept of Inorganic Chemistry, Univ of Zaragoza**

Abstract Title: **Template effect of guest cations on topology of copper-cyanide networks**
Presenting Author: **Peter Corfield, Chemistry, Fordham Univ**

Abstract Title: **Crystals structure of CFA-1, a metal organic framework (MOF) by micro electron diffraction (microED)**
Presenting Author: **Nicole Hoefer, The Ohio State University**

PL4 Fankuchen Award

David S. Goodsell
8/2/2022 @ 1:00:00 PM - 2:00:00 PM | Salon E

Abstract Title: **Art as a Tool for Structural Biology**
Presenting Author: **David Goodsell, The Scripps Research Institute and RCSB Protein Data Bank, Rutgers University**

4.2.1 Advances in xfel and Synchrotron Serial Crystallography

8/2/2022 @ 2:00:00 PM - 5:00:00 PM | Salon E
Sponsoring SIG(s): Best Pract./BioMac
Session Chair(s): Herbert J Bernstein; Aaron Brewster

This session will discuss recent advances in both xfel and synchrotron serial crystallography resulting from improvements in beamlines, detectors, data collection strategies, software and computational resources.

Abstract Title: **Chemical crystallography at XFELs: small molecule structure determination at lightning fast speeds**
Presenting Author: **Aaron Brewster, Lawrence Berkeley National Lab**

Abstract Title: **EIGER2 Upgrade: New Features for Advanced X-Ray Diffraction Experiments**
Presenting Author: **Max Burian, DECTRIS Ltd.**

Abstract Title: **Per-pixel XFEL diffraction data processing for wavelength deconvolution**
Presenting Author: **Iris Young, Lawrence Berkeley National Laboratory**

Abstract Title: **Fixed-Target Serial Crystallography at Structural Biology Center**Presenting Author: **Karolina Michalska, Argonne National Laboratory Lemont, IL**

Abstract Title: **Room Temperature Multi-Crystal Data Collection and Processing at NSLS-II Micro-Crystallography Beamlines**
Presenting Author: **Wuxian Shi, Brookhaven National Laboratory Upton, NY**

Abstract Title: **HDRMX discussion of required metadata**

Presenting Author: **Herbert Bernstein, Ronin Institute for Independent Scholarship, c/o NSLS-II, Brookhaven National Lab, Bldg 745**

4.2.2 Phase Separation & Aggregation Of Bimolecular Systems & Intrinsically Disordered Proteins

8/2/2022 @ 2:00:00 PM - 5:00:00 PM | Salons G-I
Sponsoring SIG(s): Small Angle Scattering
Session Chair(s): Richard Gillilan; Yun Liu

Many biological systems need to be studied at relatively high concentration, such as intrinsically disordered proteins and biomacromolecules in the pharmaceutical products. The discovery that liquid-liquid phase-separation (LLPS) plays a vital role in human disease has stimulated much recent research into the phase properties of concentrated solutions of biomolecules. Remarkably, it is now understood that the structural biology of proteins with intrinsically disordered regions (IDPs) is central to understanding this phenomenon. In parallel, the self-association, rheological properties and solubility limits of concentrated biologics, particularly monoclonal antibodies (mAbs), continues to be a subject of great practical importance in pharmaceuticals. The conventional use of dilute solutions by small angle scattering has already yielded important insights into the conformational changes that are associated with aggregation and LLPS behavior. Monoclonal antibody studies, on the other hand, have focused on interpreting structure factors from concentrated solutions to gain insight into intermolecular interactions. Simulations inspired by advances in Soft Materials, Colloid Science, and active matter have also played an important role in this field by incorporating ever more sophisticated particle models. This session seeks to bring together experts in this wide range of fields having common interest in concentrated or phase-separated biomolecular solutions.

Abstract Title: **Characterize the Behavior of Protein Molecules In Concentrated Environments Using Small-Angle Scattering**
Presenting Author: **Amy Xu, Louisiana State University**

Abstract Title: **Small Angle X-Ray Studies of Protein-Protein Interactions at High Concentration to Understand Viscosity, Opalescence, and Phase Separation**
Presenting Author: **William Kimball, The University of Texas at Austin**

Abstract Title: **Determining the structural ensembles of disordered RNA and proteins using an integrated approach**
Presenting Author: **Tong Wang, Cornell University**

Abstract Title: **Dynamic properties of reversible clusters in concentrated lysozyme solutions with both a short-range attraction and long-range repulsion**
Presenting Author: **Yun Liu, NIST**

Abstract Title: **Understanding intermolecular structure and forces in concentrated protein solutions through multi-protein simulations and structure factor measurements**
Presenting Author: **Richard Gillilan, CHESS, Cornell Univ**

4.2.3 Cool Structures II

8/2/2022 @ 2:00:00 PM - 5:00:00 PM | Salons A-B
Sponsoring SIG(s): Small Molecule
Session Chair(s): Dan Decato; Stacey Smith

Structure elucidation from nanometer-sized crystals has positioned microcrystal electron diffraction at the forefront of structural science. This session will feature small molecule (< 150 atoms per molecule) structures solved using MicroED and aims to highlight successes made possible by MicroED. Speakers will be selected from contributed abstracts. Submissions from students are encouraged.

Abstract Title: **Molecular Geometries of Transition Metal Complexes Influenced by Metal-Sulfur Interactions**
Presenting Author: **Kamran Ghiassi, Air Force Research Laboratory**

Abstract Title: **Copper and Manganese Coordination Complexes Synthesized via Self Assembly Using a Chiral Ligand**
Presenting Author: **Taylor Keller, Temple University Fairfield, PA**

Abstract Title: **Novel chiral aryltetraline lactone core and furo[3,4-c] pyranone structure for the synthesis of bioactive lignans and furopyranones**
Presenting Author: **Peter Mpaata, Brigham Young University**

Abstract Title: **Green Synthesis of 2-Carbamidinopyrazine**
Presenting Author: **Raúl Castañeda, New Mexico Highlands University las vegas, NM**

Abstract Title: **Structural Chemistry of Cyanoximes.**
Presenting Author: **Nick Gerasimchuk, Chemistry, Missouri State Univ.**

4.2.4 General Interest 3

8/2/2022 @ 2:00:00 PM - 5:00:00 PM | Salon C-D
Sponsoring SIG(s): General Interest
Session Chair(s): Victoria Drago; Kristofer Gonzalez-DeWhitt

Abstract Title: **Screening approaches that explore chemical space in order to identify suitable starting conditions for structure determination by cryoEM or other methods**
Presenting Author: **Patrick Shaw Stewart, Douglas Instruments Ltd**

Abstract Title: **CryoDiscovery™: Public Data-based AI/ML model enhancements for Cryo-EM Image Analysis**
Presenting Author: **Narasimha Kumar, Health Technology Innovations Portland, OR**

Abstract Title: **An Automated in situ Diffraction Platform for Serial Crystallography Studies at Room Temperature**
Presenting Author: **XIAOJING YANG, University of Illinois Chicago**

Abstract Title: **Discovery and characterization of novel ubiquitin-targeted effector proteins in pathogenic bacteria**
Presenting Author: **Jonathan Pruneda, Oregon Health & Science University**

Abstract Title: **Supramolecular landscape of bio-complex: versatility of peptide-based synthons**
Presenting Author: **Joanna Bojarska, Technical University**

Abstract Title: **Discovery of inhibitors and covalent inactivators targeting proline cycle enzymes using focused fragment-based approaches**
Presenting Author: **John Tanner, Dept of Biochemistry, Univ of Missouri Columbia**

4.2.5 Structures of Very Large Assemblies

8/2/2022 @ 2:00:00 PM - 5:00:00 PM | Salon F
Sponsoring SIG(s): cryo-EM
Co-Sponsoring SIG(s): BioMac
Session Chair(s): Andre Hoelz; Lisa Eshun-Wilson

Structural cell biology has dramatically advanced from studying individual proteins and enzymes to macromolecular assemblies of sizes with an increasing complexity–doubling about every decade over the last century. With the introduction of direct detectors, cryo-electron microscopy (cryoEM) was revolutionized and established a methodology to study massive biological assemblies that are recalcitrant to crystallization, at resolutions previously only attainable by X-ray crystallography. Moreover, focused-ion beam (FIB) milling and cryo-electron tomography (cryo-ET) now allow for the visualization of macromolecular machineries in their native cellular environments. The combination of these structural methods with improvements in traditional reconstitution biochemistry and cross-linking mass spectrometry enabled structural advances that seemed impossible less than a decade ago. In this session titled, “Structures of Very Large Assemblies”, we celebrate some of the recent spectacular advances – pushing the boundaries of larger and more complex cellular machineries, which remains a major frontier.

Abstract Title: **Architecture of the cytoplasmic face of the nuclear pore**
Presenting Author: **Si Nie, California Institute of Technology**

Abstract Title: **Structure of the human inner kinetochore bound to a centromeric CENP-A nucleosome**
Presenting Author: **Kyle Muir, MRC Laboratory of Molecular Biology**

Abstract Title: **Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7**
Presenting Author: **Luke Ferro, Whitehead Institute**

Abstract Title: **Structures of a cyanobacterial phycobilisome in the light harvesting and the quenched states**
Presenting Author: **Paul Sauer, UC Berkeley**

Abstract Title: **Structures of Tetrahymena’s respiratory chain reveal the diversity of eukaryotic core metabolism**
Presenting Author: **Maria Maldonado, University of California, Davis**

Abstract Title: **Structural analysis of Legionella pneumophila Dot/Icm type IV secretion system core complex**
Presenting Author: **Clarissa Durie, University of Missouri**

AMB All Members Business Meeting

8/2/2022 @ 5:00:00 PM - 6:00:00 PM | Salon E

BAN Art Show & Banquet

8/2/2022 @ 6:30:00 PM - 10:30:00 PM
6:30 PM PT - Ballroom Foyer
7:30 PM PT - Dinner in Salons E-F

Planning Meeting for ACA2023:

8/3/2022 @ 9:00 AM | Columbia/Willamette Room