2023

2023 ACA Annual Meeting Summary

Contents

2023 ACA ANNUAL MEETING
Full Program w/ Abstracts

ACA: The Structural Science Society
www.amercrystalassn.org

2023 Full Program w/ Abstract List

2023 ACA Meeting Committee:
B. Mercado
A. Gardberg
S. Powell
S. Smith

We are delighted to extend an invitation for you to attend the 73rd annual meeting of the American Crystallographic Association which will be held from Friday, July 7th to Wednesday, July 12th, 2023 as a fully in-person meeting. Scientists interested in biological, chemical, and material structures will travel to the waterfront in Baltimore, MD. This year's meeting will again cover a broad array of structural topics such as quantum crystallography, structural genomics, artificial intelligence and machine learning, MicroED, structure based drug design, the future of light sources, and many more. ACA values the contributions of its members from all backgrounds and we are excited for the addition of a DEI focused session to this year's program. We welcome all young scientists to our community and will be hosting a career panel for early career scientists, a Three Minute Thesis competition at ACA2023.

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/pastmeetings.

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 2023 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: Advanced Topics in Single Particle Cryo-EM & Cryo-ET

Date: Friday, July 7
Start: 9:00 AM
Room: Laurel ABCD

Workshop #2: SAMPREP (Sample Attributes for Multiple-techniques and Principal Requirements for Experiments in Pan-structural biology) Workshop

Date: Friday, July 7

Start: 8:30 AM
Room: Kent AB

Workshop #3: Structure refinement and disorder modelling with Olex2 and NoSpherA2

Date: Friday, July 7
Start: 8:00 AM
Room: Essex AB

Workshop #4: Best Practices of the Quantum-Mechanics (QM) driven Macromolecular Refinement

Date: Friday, July 7
Start: 8:50 AM
Room: Falkland

Workshop #5: Simple and Advanced Single Crystal X-Ray Structure Refinement Using ShelXle

Date: Friday, July 7
Start: 10:00 AM
Room: Essex C

First Time Attendee Meet Up

Date: Friday, July 7
Start: 5:30 PM
End: 6:30 PM
Room: Galena

Join select members of the YSIG leadership for this session, which aims to introduce first time attendees to ACA2023, provide important information, and create a vibrant sense of community right from the start. At ACA we believe in fostering an inclusive and engaging environment for all our attendees. We understand that attending a professional conference can be both exciting and overwhelming. This event is designed to help first time attendees navigate their way through the exciting opportunities and events at ACA2023. Also, did you sign up for a Meeting Mentor? Please meet your mentor here.

Welcome & Keynote

Date: Friday, July 7
Start: 6:30 PM
End: 7:30 PM
Room: Waterview ABCD

The Welcome and Keynote Address will mark the beginning of this educational and inspiring program, where the ACA Meeting Committee, President, Council Officers and our distinguished speaker, Dr. Venki Ramakrishnan will host this event to welcome everyone to ACA2023. Read more about Dr. Ramakrishnan....

Opening Reception

Date: Friday, July 7
Start: 7:30 PM
End: 10:30 PM
Room: Exhibit Hall

We cordially invite you to join us at the opening reception of ACA2023, where you can connect and network with professionals from various fields. This event provides an excellent opportunity to establish valuable connections, exchange ideas, and forge new collaborations in a relaxed and welcoming atmosphere.

Saturday, July 8, 2023 [Day #1]

TR1 From Atoms to Cells – Electron Microscopy for Structure Solution

Session Chair(s): Jim Ciston, Tamir Gonen
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Essex A-C

Structural determination in biology and materials science encompasses all resolutions, from atoms to entire organelles and cells. Knowledge of the three dimensional structure of biological materials, metals, materials and cells helps guide rational drug design and development, understanding of novel electronic materials, and understanding of the precise local structure of layered, disordered or amorphous materials. In this year's Transactions symposium of the American Crystallographic Association we put together a fantastic lineup of top scientists working on all resolution scales and a multitude of technologies that are related.

9:00 - 9:30am
191 Imaging Neurons by Cryo-Electron Tomography
Dr. Matthew T Swulius
Penn State College of Medicine, Hershey, PA, USA

9:30 - 10:00am
233 MicroED Structure of a Protoglobin Reactive Carbene Intermediate
Emma Danelius1, Nicholas J. Porter2, Johan Unge1, Frances H. Arnold2, Tamir Gonen1
1University of California Los Angeles, Los Angeles, CA, USA. 2California Institute of Technology, Pasadena, CA, USA

10:30 - 11:00am
94 Probing the atomically diffuse interfaces in core-shell nanoparticles in three dimensions
Zezhou Li1, Zhiheng Xie1, Yao Zhang1, Xilong Mu1, Jisheng Xie1, Hai-jing Yin1, Ya-wen Zhang1, Colin Ophus2, Jihan Zhou1
1Peking University, Beijing, Beijing, China. 2Lawrence Berkeley National Laboratory, Berkeley, CA, USA

11:00 - 11:30am
92 Solving 3D nanostructures using ptychographic atomic electron tomography
Colin Ophus
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

1.1.1 Alternative Methods to Predict and Solve Crystal Structures I

Session Chair(s): Luca Iuzzolino & Wenqian Xu
Sponsoring SIG(s): Small Molecule
CoSponsoring SIG(s): Industrial, Materials, Powder, Service
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Laurel CD

This session aims to showcase work involving alternative methods to traditional single crystal X-ray diffraction for predicting and solving crystal structures of small molecules. Examples include, but are not limited to, three-dimensional electron diffraction, small angle scattering, crystal structure prediction (CSP) methods, solid state NMR techniques, and structure solution from powder diffraction and total scattering data.

8:30 - 9:00am
288 Enhancing structure determination from powder X-ray diffraction data through multi-technique synergy
Professor Kenneth D M Harris
Cardiff University, Cardiff, Wales, United Kingdom

9:00 - 9:30am
316 Crystal Structure Prediction with Quadrupolar NMR Crystallography (QNMRX-CSP)
Austin Peach1,2, Carl Fleischer III1,2, Kirill Levin3, Jazmine Sanchez1,2, Sean Holmes1,2, Robert Schurko1,2
1The Florida State University, Tallahassee, FL, USA. 2National High Magnetic Field Laboratory, Tallahassee, FL, USA. 3University of Windsor, Windsor, ON, Canada

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9:30 - 10:00am
61 Predicting chemical shifts with graph neural networks
Ziyue Yang, Maghesree Chakraborty, Andrew White
University of Rochester, Rochester, NY, USA

10:30 - 11:00am
142 Pursuing Accurate Crystallography without Diffraction – NMR crystallography
James K. Harper
Brigham Young University, Provo, UT, USA

11:00 - 11:30am
63 A General Method for the Structure Determination of Amorphous Drugs by NMR
Manuel Cordova1, Pinelopi Moutzouri1, Sten O. Nilsson Lill2, Alexander Cousen3, Martin Kearns3, Stefan T. Norberg2, Anna Svensk Ankarberg2, James McCabe3, Arthur Pinon4, Staffan Schantz2, Lyndon Emsley1

1École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, -, Switzerland. 2AstraZeneca, Gothenburg, -, Sweden. 3AstraZeneca, Macclesfield, -, United Kingdom. 4University of Gothenburg, Gothenburg, -, Sweden

1.1.2 Data Analysis Software

Session Chair(s): Herbert Bernstein & Marian Szebenyi
Sponsoring SIG(s): Best Practices
CoSponsoring SIG(s): Light Sources
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Kent A-C

In this symposium we will hear from experts and pioneers in the field of electron cryomicroscopy (cryoEM). Both applications and software for cryoEM will be highlighted as new technologies are developed and described by the experts. We will explore the uses of two other cryoEM methods, namely electron cryotomography (cryoET) of synapses and neuronal networks and microcrystal electron diffraction (MicroED) for drug discovery and the determination of novel structures. Finally, we will hear about applications of scanning electron microscopy and investigations of inorganic layered, disordered or amorphous materials by diffraction methods. We will also hear about the latest and greatest from experts involved in the development of data reduction software for X-ray crystallography and MicroED.

8:30 - 9:00am
187 A decade of processing multi-modal data at XFELs
Aaron S Brewster, Daniel W Paley, Nicholas K Sauter
Lawrence Berkeley National Labs, Berkeley, CA, USA

9:00 - 9:30am
209 Reciprocal space mapping for macromolecular crystallography
Steve P Meisburger1, Nozomi Ando2
1Cornell High Energy Synchrotron Source, Ithaca, NY, USA. 2Chemistry & Chemical Biology, Cornell University, Ithaca, NY, USA

9:30 - 10:00am
52 Variational Inference for Scaling Unconventional Diffraction Data
Kevin M Dalton1, Jack B Greisman2, Doeke R Hekstra1
1Harvard University, Cambridge, MA, USA. 2D. E. Shaw Research, New York, NY, USA

10:30 - 11:00am
50 GSAS-II in 2023
Dr. Brian H. Toby, Dr. Robert B. Von Dreele
Advanced Photon Source, Argonne National Lab, Lemont, IL, USA

11:00 - 11:30am

259 SASSIE: A BioSAS Experiment Planning and Data Analysis Tool
Susan Krueger1,2, Joseph E. Curtis2
1Dept. of Materials Science and Engineering, University of Maryland, College Park, MD, USA. 2NIST Center for Neutron Resarch, NIST, Gaithersburg, MD, USA

1.1.3 Opening the Black Box of Neutrons

Session Chair(s): Jue Liu & Christina Hoffman
Sponsoring SIG(s): Neutron/Materials/Powder
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Waterview CD

Neutron scattering user facilities are a unique resource to provide broad access to the scientific community to study materials and compounds. However, many myths and “rules of thumbs” for neutron experiments around. This session aims to give background information for the novice and the experienced user to plan experiments, manage resources and expectations for data reduction and analysis. All steps of the process are highly dependent on the technique and the knowledge of an instrument responsible scientist.

8:30 - 8:50am
208 Advances in Single Crystal Neutron Diffraction
christina hoffmann
ORNL, oak ridge, tn, USA

8:50 - 9:10am
198 Structure and dynamics in BaTiS3 hexagonal perovskite as seen by neutron scattering
Dr Raphael P Hermann, Dr George Yumnam, Dr Michael Michael E Manley, Dr Barry L Winn, Dr Christina Hoffmann
Oak Ridge National Laboratory, Oak Ridge, TN, USA

9:10 - 9:30am
148 Solving the magnetic structures in the complex in-field phase diagram of YMn6Sn6−xGex using single crystal neutron diffraction
Rebecca L Dally1, Hari Bhandari2,3, Peter E Siegfried2,3, Resham Regmi2,3, Kirrily C Rule4, Songxue Chi5, Igor I Mazin2,3, Jeffrey W Lynn1, Nirmal J Ghimire2,3
1NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, USA. 2Department of Physics and Astronomy, George Mason University, Fairfax, VA, USA. 3Quantum Science and Engineering Center, George Mason University, Fairfax, VA, USA. 4Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW, Australia. 5Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

9:30 - 9:45am

260 Recent Development of Operando Neutron Diffraction and Its Application in Studying Energy Storage Materials
Dr Jue Liu, Dr Zhijia Du, Dr Michelle Everrett
Oak Ridge National Lab, Oak Ridge, TN, USA

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9:45 - 10:00am
121 Where the H is the interstitial: Single crystal neutron diffraction studies of complex metal hydrides
Dr. Christina Hoffmann1, Dr. Xiaoping Wang1, Dr. Susan E. Latturner2
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2Florida State University, Tallahassee, FL, USA

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10:30 - 10:50am
300 Adsorption and separations processes within metal-organic frameworks through neutron scattering
Dr Craig M Brown1, Dr Hayden Evans2, Dr Malia Wenny2, Dr Ryan Klein3
1NIST, Gaithersburg, MS, USA. 2NIST, Gaithersburg, MD, USA. 3NREL, Golden, Co, USA

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10:50 - 11:10am
196 Depth-Sensitive Grazing Incidence Crystallography: From Atomic to Mesoscopic Scale In-plane Structures
Dr Valeria Lauter
ORNL, Oak Ridge, TN, USA

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11:10 - 11:30am
299 Operando Small Angle Neutron Scattering and its Applications in Energy Storage Materials
Dr. Lilin He
Oak Ridge National Laboratory, Oak Ridge, TN, USA

1.1.4 General Interest I

Session Chair(s): Tim Stachowski & Charles Bou-Nader
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Laurel AB

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

9:00 - 9:30am
177 Structural basis of dsRNA recognition by the J2 monoclonal antibody
Charles Bou-Nader1, Ankur Bothra2, Ilias Skeparnias1, David N. Garboczi3, Stephen H. Leppla2, Jinwei Zhang1

1Laboratory of Molecular Biology, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, USA. 2Laboratory of Parasitic Diseases, National Institute of Allergy and Infectious Diseases, Bethesda, MD, USA. 3Structural Biology Section, Research Technologies Branch, National Institute of Allergy and Infectious Diseases, Bethesda, MD, USA

9:30 - 10:00am
160 Using X-ray footprinting to investigate dose rate effects on oxidative damage to proteins
Sayan Gupta, Jamie Inman, Antoine Snijders, Corie Ralston
Lawrence Berkeley National Lab, Berkeley, CA, USA

10:30 - 10:50am
228 Structural and Biochemical Investigation of a Novel Natural Product Amination Domain
Michael R Rankin1,2, Dr. Dheeraj Khare1, Estefanía Martínez Valdivia1,3, Dr. David H Sherman1,3,4,5,6, Dr. William H Gerwick7,8, Dr. Anna K Mapp1,3,6, Dr. Janet L Smith1,2,3
1Life Sciences Institute, University of Michigan, Ann Arbor, MI, USA. 2Department of Biological Chemistry, University of Michigan Medical School, Ann Arbor, MI, USA. 3Program in Chemical Biology, University of Michigan, Ann Arbor, MI, USA. 4Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI, USA. 5Department of Microbiology & Immunology, University of Michigan, Ann Arbor, MI, USA. 6Department of Chemistry, University of Michigan, Ann Arbor, MI, USA. 7Center for Marine Biotechnology and Biomedicine, Scripps Institution of Oceanography, San Diego, CA, USA. 8Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA, USA

10:50 - 11:10am
376 Structures of Langya virus fusion protein ectodomain in pre and post fusion conformation
Aaron J May, Karunakar Pothula, Katarzyna Janowska, Priyamvada Acharya
Duke University, Durham, North Carolina, USA

11:10 - 11:30am
279 MetalJet X-ray sources for experiments at non-ambient pressures
Dr. Julius Hållstedt1, Rob Drake2, Geethanjali Gopakumar1, Emil Espes1
1Excillum, Kista, -, Sweden. 2PROTO Manufacturing Ltd, LaSalle, Ontario, Canada

1.1.5 Crystal Growth & Optimization

Session Chair(s): Gabby Budziszewski & Xu Liu
Sponsoring SIG(s): Biological Macromolecules, Small Molecule
CoSponsoring SIG(s): Best Practices
Date: Saturday, July 8
Start: 8:30 AM
End: 11:30 AM
Room: Waterview AB

For most macromolecules and small molecules, the art of crystal growth is still largely determined experimentally and typically involves iterative optimization steps to produce appropriate diffraction-

quality crystals. This session welcomes abstract submissions that include insights into crystal growth optimization, crystal growth prediction, co-crystallization and soaking, and strategies to influence crystal morphologies.

8:35 - 9:00am
78 RNA Crystal Improvement with Definitive Screening Designs
Dr Barat S. Venkataramany1, Dr Franics A Acquah1, Mr Syed A Aslam1, Professor Charles W Carter, Jr.2, Associate Professor Blaine H M Mooers1,3,4
1Department of Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA. 2Biochemistry and Biopysics, University of North Carolina School of Medicine, Chapel Hill, NC, USA. 3Laboratory of Biomolecular Structure and Function, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA. 4Stephenson Cancer Center, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

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9:00 - 9:25am
155 A comprehensive strategy for efficient generation of well-diffracting crystals
Dr. Miki Senda, Prof. Toshiya Senda
High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan

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9:25 - 9:50am
19 Computational Protein Engineering for Systematic Enhancement of Crystallization Propensity
Nooriel E Banayan, Blaine Loughlin, Dr. Shikha Singh, Dr. Farhad Forouhar, Dr. John F Hunt
Columbia University, New York, NY, USA

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10:30 - 10:50am
137 Encapsulated Nanodroplet Crystallisation of Small Molecules (ENaCt): High-throughput Small-scale Crystallisation Methods Direct to Single Crystal XRD
Dr Michael J Hall
Newcastle University, Newcastle upon Tyne, Tyne and Wear, United Kingdom. Indicatrix Crystallography, Newcastle upon Tyne, Tyne and Wear, United Kingdom

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10:50 - 11:10am
345 Crystallizing Student-Interest in Biochemistry
Susanna Huang1,2, Selina Huang1
1SeNA Research Institute, Atlanta, GA, USA. 2Georgia Institute of Technology, Atlanta, GA, USA

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11:10 - 11:30am
33 Crystal growth and physical properties of EuIr3Si7 single crystal
Dr Binod Kumar Rai
Savannah River National Laboratory, Aiken, SC, USA

YSIG Lunch w/ Dr. Ramakrishnan [Registration Required]

Date: Saturday, July 8
Start: 11:30 AM

End: 1:00 PM
Room: Dover A-B

Join us for a buffet lunch and following the lunch, Dr. Venki Ramakrishnan will be available to personally sign copies of "Gene Machine." This is an exceptional chance to interact with the author and gain unique insights into his work and incredible accomplishments. We invite YSIG members to join us for free and for any other level of membership, the cost for the lunch is $100 UDS. Registration is required by anyone wanting to attend (registration will close on June 23) and we encourage attendees to bring copies of "Gene Machine" as we will not have any onsite for purchase. This lunch is graciously sponsored in part by the American Institute of Physics.

TMT 3 Minute Thesis Competition

Date: Saturday, July 8
Start: 1:00 PM
End: 2:00 PM
Room: Essex A-C

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

11 Structural basis of DNA binding by the NAC transcription factor ORE1, a master regulator of plant senescence
Inseop Chun1, Hyo Jung Kim2, Sunghyun Hong3, Yeon-Gil Kim4, Min-Sung Kim5
1Postech, pohang-si, Gyeongbuk, Korea, Republic of. 2center for plant aging Research, Institute for Basic Science, Daegu, Gyeongbuk, Korea, Republic of. 3center for genome Engineering, institute for Basic Science, Daejeon, Chungbuk, Korea, Republic of. 4Pohang Accelerator Lab, POSTECH, Pohang, Gyeongbuk, Korea, Republic of. 5Postech, Pohang, Gyeongbuk, Korea, Republic of

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36 A combined structural, spectroscopic, electrochemical, and magnetic study of Nickel(II) pyrazolates: dinuclear [Ni2], linear [Ni3], and triangular [Ni3] incorporating five-/six-coordinate Ni2+ ions.
Zhichun Shi1, Dr Indranil Chakraborty1, Prof Yiannis Sanakis2, Prof Raphael G Raptis1
1Florida International University, Chemistry Department, Miami, FL, USA. 2Institute of Nanoscience and Nanotechnolgy, National Centre of Scientific Research “Demokritos”, Aghia Paraskevi, Attiki, Greece

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349 Improving Data Collection Efficiency in small-molecule Serial Femtosecond Crystallography at X-ray Free Electron Lasers
Ms. Elyse A Schriber1, Dr. Daniel Paley2, Dr. Raymond Sierra3, Dr. Aaron Brewster2, Prof. James N. Hohman4

1Institute of Materials Science, University of Connecticut, Storrs, CT, USA. 2Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 3Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. 4Department of Chemistry, University of Connecticut, Storrs, CT, USA

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278 Electron Diffraction – The Swiss knife among the analytical equipment for solid state characterization for pharmaceuticals

Danny Stam, Dr. Johannes Merkelbach, Dr. Christian Jandl
ELDICO Scientific AG, Villigen, Argau, Switzerland

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225 Increasing completeness in single-crystal high-pressure diffraction experiments by pre-orienting crystals

Dr Daniel M Tchoń1, Aleksandra Zwolenik2, Dr hab. Anna M Makal2
1Molecular Biophysics and Integrated Bioimaging, Lawrence Berkeley National Laboratory, Berkeley, California, USA. 2Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, Mazovia, Poland

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157 Probing Pressure-Driven Protein Phase Behavior via In-Situ High-Pressure Scattering Methods

Brian Paul1,2, Susana CM Teixeira1,2, Eric M Furst1, Abraham M Lenhoff1, Norman J Wagner1
1University of Delaware, Newark, Delaware, USA. 2NIST Center for Neutron Research, Gaithersburg, Maryland, USA

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75 Quality Assessment and Biomolecular Structure Modeling for Cryo-EM using Deep Learning

Genki Terashi, Xiao Wang, Tsukasa Nakamura, Devashish Krishna Prasad, Daisuke Kihara
Purdue University, West Lafayette, Indiana, USA

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62 CryoFAST™: Automated Cryo-Electron Microscopy Data Acquisition using Machine Learning

Mr Elliot Gray1, Dr Dmitry Lyumkis2, Dr Atousa Mehrani2, Mr Narasimha Kumar1
1HTI Inc, Portland, Oregon, USA. 2Salk Institute, La Jolla, California, USA

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51 Solution characterization of the dynamic conjugative entry exclusion protein TraG

Nicholas J Bragagnolo, Dr. Gerald F Audette
York University, Toronto, Ontario, Canada

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46 Refinement of crystal structures at ultralow resolution with assistance from AlphaFold modeling and Rosetta optimization

Wei Wang, Wayne A Hendrickson
Columbia University, New York, NY, USA

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19 Computational Protein Engineering for Systematic Enhancement of Crystallization Propensity

Nooriel E Banayan, Blaine Loughlin, Dr. Shikha Singh, Dr. Farhad Forouhar, Dr. John F Hunt
Columbia University, New York, NY, USA

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356 Mode of Substrate Binding for Ketohexokinase across Isozymes and Species Implies an Induced-Fit mechanism

Miss So Young Bae, Professor of Biology Karen N Allen, Professor of Biology Dean R. Tolan
Boston University, Boston, MA, USA

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348 Selenium Nucleic Acids for Innovative Structural Biology
Professor Zhen Huang, Doctor Ziyuan Fang, Student Susanna Huang
SeNA Research Institute, Atlanta, GA, USA

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347 Single Selenium Atom to Control Nucleic Acid Conformation and Large Crystal Growth
Professor Zhen Huang, Doctor Cen Chen, Doctor Ziyuan Fang, Student Susanna Huang, Student Selina Huang
SeNA Research Institute, Atlanta, GA, USA

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247 Filament formation drives catalysis of glutaminase
Shi Feng, Cody Aplin, Thuy-Tien T. Nguyen, Richard A. Cerione
Cornell University, Ithaca, NY, USA

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181 Preservative-induced micelle formation of poloxamer 188
Dr. Rachel R Ford
NIST Center for Neutron Research, Gaithersburg, MD, USA

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159 Structure of the catalytically active APOBEC3G bound to a DNA oligonucleotide inhibitor reveals tetrahedral geometry of the transition state
Atanu Maiti1, Adam K Hedger2,3, Wazo Myint1, Vanivilasini Balachandran1, Jonathan K Watts4,3, Celia A Schiffer4, Hiroshi Matsuo1
1Cancer Innovation Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MD, USA. 2Institute for Drug Resistance and Department of Biochemistry and Molecular Biotechnology, University of Massachusetts Chan Medical School,, Worcester, MA, USA. 3RNA Therapeutics Institute, University of Massachusetts Chan Medical School, Worcester, MA, USA. 4Institute for Drug Resistance and Department of Biochemistry and Molecular Biotechnology, University of Massachusetts Chan Medical School, Worcester, MA, USA

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73 Synthesis and Characterization of Potentially Catalytic Tolunitrile Adducts of Rhodium(II) Acetate
Malachi O Cope, Dr. Cassandra T Eagle, Alain M Beauparlant
East Tennessee State University, Johnson City, TN, USA

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44 Exploring the limits of 2D template matching for detecting targets in cellular cryo-EM images
Kexin Zhang
The University of Massachusetts Chan Medical School, Worcester, Massachusetts, USA

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39 Structural and functional divergence of a "new" class of phoshoenolpyruvate carboxykinase - insights into allosteric regulation via oligomeric changes
Dr. Matthew J McLeod1, Siddhi Balamurali1, Dr. Robert Thorne1, Dr Todd Holyoak2
1Cornell, Ithaca, New York, USA. 2University of Waterloo, Waterloo, Ontario, Canada

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344 Copper Acetate Small Molecule Crystallography Undergraduate Experiments
Mr. Alain M Beauparlant, Dr. Sandy Eagle, Mr. Malachi o Cope, Ms. Alandria R Marshall
East Tennessee State University, Johnson City, TN, USA

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499 Tetrakis(acetato) dirhodium(II), [Rh2(O2CCH3)4],
Alain Beauparlant
East Tennessee State University, Johnson City, TN, USA

TR2 From Atoms to Cells – Electron Microscopy for Structure Solution

Session Chair(s): Jim Ciston & Tamir Gonen
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Essex A-C

Structural determination in biology and materials science encompasses all resolutions, from atoms to entire organelles and cells. Knowledge of the three dimensional structure of biological materials, metals, materials and cells helps guide rational drug design and development, understanding of novel electronic materials, and understanding of the precise local structure of layered, disordered or amorphous materials. In this year's Transactions symposium of the American Crystallographic Association we put together a fantastic lineup of top scientists working on all resolution scales and a multitude of technologies that are related.

234 New cryoEM Methods to capture endogenous complexes in multiple functional states at atomic resolution
Professor Hong Hong Zhou
University of California, Los Angeles, Los Angeles, California, USA

2:30 - 3:00pm
189 New methodologies for preparing and imaging cryo-EM samples.
Gan Li1,2, Michael S Westphall2, Mr Austin Z. Salome2, Kenneth W Lee2, Joshua J Coon2,1, Timothy Grant1,2
1Morgridge Institute for Research, Madison, WI, USA. 2UW-Madison, Madison, WI, USA

3:30 - 4:00pm
382 Amino Acid Sensation and Transport by SLC38A9
Xuelang (Maymay) Mu1,2, Hsiang-Ting Lei3, Johan Hattne4,3, Tamir Gonen4,3
1• Departments of Biological Chemistry and Physiology, David Geffen School of Medicine, University of California, Los Angeles, California, USA. 2• Howard Hughes Medical Institute, University of California, Los Angeles, Los Angeles, California, USA. 3Howard Hughes Medical Institute, University of California, Los Angeles, Los Angeles, California, USA. 4Departments of Biological Chemistry and Physiology, David Geffen School of Medicine, University of California, Los Angeles, Los Angeles, California, USA

4:00 - 4:30pm
7 The National Center for CryoEM Access and Training - Establishing a cross-facility accepted training curriculum
Edward Eng, Elina Kopylov, Charlie Dubbeldam, Cathleen Castello, Christina Zimanyi
New York Structural Biology Center, New York, NY, USA

1.2.1 Exploring structure through complex modeling of multimodal experiments

Session Chair(s): Wenqian Xu, Ben Frandsen
Sponsoring SIG(s): Neutron/Materials/Powder
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Kent A-C

As the structural complexity of technologically and scientifically relevant materials increases, so too must the sophistication of structural characterization strategies increase. An important trend in this direction has recently emerged in the form of multimodal structural studies, in which multiple experimental and simulation techniques and analysis methods are combined synergistically to provide a comprehensive picture of the structure, ranging from local structure to microstructure to average structure, and from surface to bulk. This type of coordinated, coherent approach to utilizing complementary probes can provide far more information than would be available from individual probes considered in isolation. This session provides a forum for the latest developments in multimodal structural studies. Abstracts are welcome from all fields of science that involve structural characterization with diffraction, spectroscopy, scattering, microscopy techniques, and beyond. Research that employs novel experimental design or simultaneous use of multiple probes in a single experiment will be highlighted.

2:00 - 2:20pm
246 Realizing autonomous, real-time, AI-driven multimodal studies at x-ray light sources
Dr. Daniel Olds1, Dr. Phil Maffettone1, Dr. Bruce Ravel2, Dr. Thomas Caswell1, Dr. Stuart Campbell1, Dr. Howie Joress2
1Brookhaven National Laboratory, Upton, NY, USA. 2National Institute of Standards and Technology, Gaithersburg, MD, USA

2:20 - 2:40pm
346 Image Segmentation and Advanced Processing of 2D Diffraction Data
Wenqian Xu, Howard Yanxon, James Weng, Nicholas Schwarz, Uta Ruett
Argonne National Laboraotry, Lemont, IL, USA

2:40 - 3:00pm
15 Synthesis and Structural investigation of novel Barium Molybdenum Hollandite structures.
Eslam E Elbakry, Dr Jared M Allred
University of Alabama, Tuscaloosa, Alabama, USA

3:30 - 3:55pm

179 Resolving correlated reaction pathways: A multimodal analytical toolkit
Karena W Chapman
Stony Brook University, Stony Brook, NY, USA

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3:55 - 4:15pm
6 Disruption of a Key H-bond Network Dissociates Glucocorticoid Receptor-Mediated Drug Efficacy from Side Effects for Anti-Inflammation Treatment
Xu Liu
Emory Uniersity, Atlanta, GA, USA

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4:15 - 4:35pm
340 Refinement of anomalous dispersion parameters - more than model improvement
Dr. Michael Bodensteiner
University of Regensburg, Regensburg, Bavaria, Germany

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4:35 - 4:50pm
100 Complex Host Structures and Phase Transitions in Fast Charging Lithium-ion Battery Anodes from Diffraction and Complementary Techniques
Kent Griffith
UC San Diego, La Jolla, CA, USA

1.2.2 Complementary methods to study metalloenzymes

Session Chair(s): Gloria Borgstahl & Nicholas Schnicker
Sponsoring SIG(s): Biological Macromolecules
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Laurel AB

Metalloproteins are involved in many critical cellular processes, and around one-third of all proteins in nature use at least one metal ion. In addition to the typical experimental techniques used to study metalloproteins, recently, there have been considerable advances in deep/machine learning and other computational-based approaches to investigate metalloproteins. This session will highlight the complementary experimental and computational methods used to understand the fascinating mechanisms of metalloproteins.

2:00 - 2:30pm
216 Designing a Rieske Route for C-H Bond Functionalization
Jiayi Tian, Alejandro A Garcia, Jennifer Bridwell-Rabb
University of Michigan, Ann Arbor, MI, USA

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2:30 - 3:00pm
242 Challenges and Successes in Determining the Structure of Arginyltransferase 1 (ATE1)
Aaron T. Smith

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

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3:30 - 3:53pm
118 Structural and spectroscopic investigations of metal-bound rubrerythrin from B. pseudomallei
Sarah EJ Bowman1,2, Gabrielle R Budziszewski1, M Elizabeth Snell1, Tiffany R Wright1, Miranda L Lynch1, Diana CF Monteiro1
1Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA. 2University at Buffalo, Buffalo, NY, USA

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3:53 - 4:16pm
321 The Mythical Metal – Insights on the Accuracy of Metal Identification in Structural Biology
Dr Edward H Snell1,2, Dr. Elspeth F Garman3, Dr. Geoff W Grime4, Dr. Aina E Cohen5, Dr. Sarah EJ Bowman1,2
1Hauptman-Woodward Medical Research Institution, Buffalo, NY, USA. 2University at Buffalo, Buffalo, NY, USA. 3Oxford University, Oxford, N/A, United Kingdom. 4Surrey Ion Beam Center, Surrey, N/A, United Kingdom. 5Stanford Synchrotron Radiation Lightsource, Stanford, California, USA

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4:16 - 4:38pm
79 Visualization of the human manganese superoxide dismutase product inhibition mechanism and protonation states
Jahaun Azadmanesh1, Katelyn Slobodnik1, William E. Lutz1, Leighton Coates2, Kevin L. Weiss2, Dean A. A. Myles2, Thomas Kroll3, Gloria E. O. Borgstahl1
1University of Nebraska Medical Center, Omaha, NE, USA. 2Oak Ridge National Laboratory, Oak Ridge, TN, USA. 3SLAC National Accelerator Laboratory, Menlo Park, CA, USA

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4:38 - 5:00pm
105 Identifying metal redox states through low dose measurements for spatially resolved anomalous dispersion refinement
Dr. Frank Lennartz1, Dr. Jae-Hun Jeoung2, Prof. Dr. Holger Dobbek2, Dr. Manfred Weiss1
1Helmholtz-Zentrum Berlin für Materialien und Energie, , Macromolecular Crystallography, Berlin, Berlin, Germany. 2Institut für Biologie, Strukturbiologie/Biochemie, Humboldt-Universität zu Berlin, Berlin, Berlin, Germany

1.2.3 Creating Function Through Intentional Solid-State Structural Design. A James A. Ibers Memorial Session

Session Chair(s): Jim Kaduk & Danielle Gray
Sponsoring SIG(s): Small Molecule
CoSponsoring SIG(s): Industrial, Canadian
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Waterview AB

James A. Ibers (9 June 1930 – 14 December 2021) worked at the Shell Development Company and Brookhaven National Labs before ultimately landing at Northwestern University as a full professor in 1965 where he spent the entirety of his academic career. He never considered himself a crystallographer, but always an inorganic chemist who happened to use crystallography as a tool to understand structure, bonding and function of compounds and materials. His career as an inorganic chemist spanned many areas including coordination chemistry, hydrogen bonding in solids, coordination clusters, and solid-state compounds. Towards the end of his career, he concentrated on the solid-state chemistry of uranium and neptunium chalcogenides and pnictides. He was particularly interested in tellurium and its propensity to form chains in solids. Te, however, can also have intermediate "bond" lengths that are not quite a bond and yet not long enough to be considered non-bonding. This makes Te an interesting atom that often leads to difficulty with charge balancing. Ultimately Jim built his career on examining structure to understand function with the ability to one day use rational design in creating new functional solid-state materials. He held many honors including being a member of U.S. National Academy of Sciences and a member of the American Academy of Arts and Sciences. His awards include the Linus Pauling Medal, the Luigi Sacconi Medal, the Bailar Medal, and of course he was our own ACA Martin J. Buerger Awardee in 2002. Jim would not want us to focus an entire session on his accomplishments but would rather see his influence on trying to create function through intentional structural design. To read more about Jim and his amazing accomplishments check out the ACA history page...

2:00 - 2:20pm
158 James Ibers, One of the Pioneers of Modern Crystallography
Professor Carolyn P Brock
University of Kentucky, Lexington, KY, USA

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2:20 - 2:40pm
329 Site occupancy and disorder effects on Mg1−xCoxPS3 obtained through metal ionexchange metathesis
Hector C Mandujano, Dr. Tianyu Li, Dr. Peter Y Zavalij, Profesor Efrain E Rodriguez
University of Maryland, College Park, MD, USA

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2:40 - 3:00pm
77 Solid-State Form Design in Drug Product Development
Dr Rajni Miglani Bhardwaj
Molecular Profiling and Drug Delivery, Development Sciences, AbbVie, North Chicago, Illinois, USA

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3:30 - 3:55pm
54 Materials Discovery through Machine Learning: Experimental Validation and Interpretable Models
Dr Arthur Mar
University of Alberta, Edmonton, AB, Canada

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3:55 - 4:20pm
193 Ionothermal Synthesis and Characterization of Transition-Metal Thiophosphates: Ideas vs. Reality

Jason A Cody
Lake Forest College, Lake Forest, IL, USA

4:20 - 4:40pm
156 A Race Against Time: Crystallization and Characterization of Berkelium and Californium Compounds
Prof Thomas Albrecht-Schoenzart
Colorado School of Mines, Golden, CO, USA

4:40 - 5:00pm
66 Resolving crystal selection processes during optical floating zone crystal growth – novel non-destructive synchrotron and software tools for rapid grain tracking
Yusu Wang1, Songsheng Tao2, Jonathan J. Denney1, Lucas A. Pressley3, Dario C. Lewczyk1, Satya K. Kushwaha3, Mojammel Alam Khan3, Mehmet Topsakal4, Simon J. L. Billinge2,4, Peter G. Khalifah1,4
1Stony Brook University, Stony Brook, NY, USA. 2Columbia University, New York, NY, USA. 3Johns Hopkins University, Baltimore, MD, USA. 4Brookhaven National Laboratory, Upton, NY, USA

1.2.4 Small Angle Scattering To Characterize Structurally Complex Materials

Session Chair(s): Tom Fitzgibbons, Lilin He
Sponsoring SIG(s): Small Angle Scattering
CoSponsoring SIG(s): Neutrons, Industrial, Materials, Canadian
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Waterview CD

Complex materials exhibit hierarchical structures with unique geometries. Structural characterization of such materials is extremely challenging. Small angle scattering, often combined with wide angle scattering and modeling approaches have been playing an essential role in elucidating many of these complex structures. In this session we will discuss recent advances in the characterization of complex geometric systems such as polymers, ceramics, porous materials, lyotropic liquid crystals, and other hierarchical systems formed through self-assembly or multicomponent interactions. The structure that exists within these systems and at their interfaces govern the observed macroscopic properties of the material. Gaining this understanding and therefore control of the structure and interfacial properties will allow for the rational design of new materials for applications ranging from energy storage, gas capture, water purification to food science.

2:00 - 2:15pm
385 Chain Growth Kinetics of Conjugated Polymers on Ferromagnetic Nanoparticles Investigated by SANS
Sofia Fanourakis1, Debora Rodrigues1, Sharona Barroga2, Jem Perez3
1University of Houston, Houston, TX, USA. 2University of the Philippines,, Diliman, Quezon City, Philippines. 3University of the Philippines, Diliman, Quezon City, Philippines

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2:15 - 2:30pm
365 A SAXS/WAXS study: structural reconstruction and evolution of nanoparticle assemblies
Ruipeng Li
Brookhaven National Lab, Upton, NY, USA

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2:30 - 3:00pm
389 Computational Reverse Engineering Analysis of Scattering Experiments (CREASE) for Soft Materials
Prof. Arthi Jayaraman
University of Delaware, Newark, DE, USA

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3:30 - 3:55pm
194 Mapping of pathological inclusions in human brain tissue with Alzheimer's disease
Abdullah Al Bashit1, Prakash Nepal1, Lee Makowski1, Lin Yang2
1Northeastern University, Boston, MA, USA. 2Brookhaven National Laboratory, Upton, NY, USA

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3:55 - 4:10pm
119 X-ray scattering tomography for visualizing cellulose in plants
Lin Yang
Brookhaven National Laboratory, Upton, NY, USA

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4:10 - 4:25pm
297 Hierarchical structure of cellulose microfibrils for regenerated cellulose fiber
Dr. Jiliang Liu
ESRF, Grenoble, Alps, France

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4:25 - 4:55pm
373 Hierarchical Structures of Polysaccharides
Dr. Yimin Mao
University of Maryland, College Park, College Park, MD, USA. National Institute of Standards and Technology, Gaithersburg, MD, USA

1.2.5 Alternative Methods to Predict and Solve Crystal Structures II

Session Chair(s): Luca Iuzzolino & Wenqian Xu
Sponsoring SIG(s): Small Molecule
CoSponsoring SIG(s): Industrial, Materials, Powder, Service
Date: Saturday, July 8
Start: 2:00 PM
End: 5:00 PM
Room: Laurel CD

This session aims to showcase work involving alternative methods to traditional single crystal X-ray diffraction for predicting and solving crystal structures of small molecules. Examples include, but are not

limited to, three-dimensional electron diffraction, small angle scattering, crystal structure prediction (CSP) methods, solid state NMR techniques, and structure solution from powder diffraction and total scattering data.

2:00 - 2:30pm
47 CRYSTAL STRUCTURES OF LARGE-VOLUMECOMMERCIAL PHARMACEUTICALS
James A Kaduk1, Tawnee M Ens1, Nicolas C Boaz1, Anja Viera Dosen2, Thomas N Blanton2
1North Central College, Naperville, IL, USA. 2ICDD, Newtown Square, PA, USA

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2:30 - 3:00pm
140 In-situ studies of molecular copper compounds for highly selective purification of ethylene
Prof. Peter W. Stephens1, Prof. Rasika H.V. Dias2, Dr. Andrey A Yakovenko3
1Stony Brook University, Stony Brook, NY, USA. 2University of Texas, Arlington, TX, USA. 3Argonne National Laboratory, Lemont, IL, USA

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3:30 - 4:00pm
10 Combining techniques for increased accuracy of crystal structures from powder diffraction data
Dr. Dubravka Sisak Jung1, Dr. Stipe Lukin2, Dr. Ivan Halasz2
1DECTRIS, Baden, Aargau, Switzerland. 2Institute Ruder Boskovic, Zagreb, Croatia, Croatia

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4:00 - 4:30pm
166 Combining modern structural tools to solve a tough lithium-tantalum-oxide problem; MicroED, laboratory and synchrotron X-ray, and DFT.
Lee M Daniels1, James A Kaduk2,3, Joseph D Ferrara1, Winnie Wong-Ng4, Amrit P Kafle5, Colin W Scherry3
1Rigaku Americas Corp, The Woodlands, TX, USA. 2Illinois Institute of Technology, Chicago, IL, USA. 3North Central College, Naperville, IL, USA. 4NIST, Gaithersburg, MD, USA. 5Catholic University of America, Washington, DC, USA

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4:30 - 5:00pm
222 Accurate crystal structures of ices from X-ray and ED with Hirshfeld atom refinement
Prof Krzysztof Wozniak1, Dr Michal Chodkiewicz1, Dr Roman Gajda1, Prof Vitali B Prakapenka2, Prof Przemyslaw Dera3
1University of Warsaw, Warszawa, Mazovia, Poland. 2APS, Argonne National Laboratory, Lermont, IL, USA. 3Université d'hawaï à mānoa, Honolulu, HI, USA

Poster Session #1

Date: Saturday, July 8
Start: 5:30 PM
End: 7:30 PM
Room: Exhibit Hall

We are delighted to invite you to the first of three engaging and insightful poster sessions. The poster session promises to be a vibrant and dynamic event, offering you the chance to engage directly with

presenters, ask questions, and delve deeper into their work. This interactive format allows for meaningful discussions and fosters collaborations among participants. The poster session will be complemented by light refreshments, creating a relaxed and informal atmosphere conducive to networking. It's an ideal setting to meet fellow attendees, expand your professional network, and forge new connections within your field of interest. We also encourage you to visit our vendors located throughout the exhibit show area.

39 Structural and functional divergence of a "new" class of phoshoenolpyruvate carboxykinase - insights into allosteric regulation via oligomeric changes
Dr. Matthew J McLeod1, Siddhi Balamurali1, Dr. Robert Thorne1, Dr Todd Holyoak2
1Cornell, Ithaca, New York, USA. 2University of Waterloo, Waterloo, Ontario, Canada

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419 BICALUTAMIDE POLYMORPHISM: SOLID-STATE NMR CHARACTERIZATION OF TWO CRYSTALLINE FORMS
Miss Shubha Gunaga, Miss Janice Rusli, Prof. David L. Bryce
University of Ottawa, Ottawa, Ontario, Canada

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434 Dissecting M5717 killing of malaria parasites
Ms. Meseret Haile1, Ms. Jing Cheng1, Dr. Leonie Anton1, Dr. David Cobb2, Ms. Carolyn Lee1, Dr. Chi-Min Ho1
1Columbia University, New York, NY, USA. 2Columbia University*, New York, NY, USA

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399 Understanding preferences for double-stranded RNA cleavage by SARS-CoV-2 enzyme nsp15
Dr. Zoe M Wright, Mr. Kevin John U Butay, Ms. Isha M Wilson, Dr. Geoff A Mueller, Dr. Mario J Borgnia, Dr. Robin E Stanley
NIEHS, Durham, NC, USA

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406 Structural basis and inhibition of outer membrane protein biogenesis in pathogenic Neisseria
Evan Billings1, Dr. Richard Stein2, Natalie Wolske3, Carsten Seyfert4, Dr. Hassane Mchaourab2, Dr. Aleksandra Sikora3, Dr. Rolf Muller4, Dr. Nicholas Noinaj1
1Purdue University, West Lafayette, IN, USA. 2Vanderbilt University, Nashville, TN, USA. 3Oregon State University, Cornwallis, OR, USA. 4Helmholz Institute for Pharmaceutical Research, Saarbrucken, Saarland, Germany

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405 Building ground truth benchmarks of structural heterogeneity for cryo-EM
Dr. Andrew V. Grassetti, Laurel F. Kinman, Dr. Joseph H. Davis
Massachusetts Institute of Technology, Cambridge, MA, USA

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274 cryoHub: A user-friendly, web-based platform for command-line scientific research tools specializing in cryo-EM analysis
Le Yang1, Chuteng Li2, Han Liu3, Rong Xiao3, Benjamin Walls4, Yicheng Zhang1, Jiawen Zhang1, Lueyu Wang1, Chuck Lugai5, Sujit Lakshmikanth1, Nicholas Vangos1, Dr. Michael Cianfrocco1, Dr. Yilai Li1

1University of Michigan, Ann Arbor, MI, USA. 2University of Washington, Seattle, WA, USA. 3Virginia Polytechnic Institute and State University, Blacksburg, VA, USA. 4Northeastern University, Boston, MA, USA. 5Pomona College, Claremont, CA, USA

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199 Structural characterization of a zinc-coordinated bis-histidine heme-binding site in the DUF2470 cyanobacterial protein

Estella F. Yee1, Kriti Chopra1, Nicolas Grosjean2, Desigan Kumaran1, Macon Abernathy3, James Byrnes1, Lin Yang1
1Brookhaven National Lab, Upton, NY, USA. 2Joint Genome Institute, Berkeley, CA, USA. 3Stanford Synchrotron Radiation Lightsource, Menlo Park, CA, USA

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48 Structural basis for the viral hijacking of Phosphoribosylformylglycinamidine Synthase

Nandini ., Jarrod B. French
The Hormel Institute, University of Minnesota, Austin, MN, USA

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426 A disulfide bridge survey and library

Christopher J Williams, Sushrit Pasumarthy, Jane S Richardson
Duke University, Durham, NC, USA

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439 Structure determination of outer surface protein BBA57 from the Lyme disease pathogen support the structure-based design of needed therapeutics

Jeyatharshika Antonyrajah1,2, Dr. Matthew R Goode1,2, Dr. Emily K Kaschner1,2, Dr. Debra T Hansen2, Dr. Petra Fromme1,2
1Arizona State University, Tempe, Arizona, USA. 2Biodesign Center for Applied Structural Discovery, Tempe, Arizona, USA

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423 Structural Studies of Secreted Autotransporter Toxin, A Serine-Protease Autotransporter of Enterobacteriaceae

Mr Dalton E Kiefer, Dr. Jose Meza-Aguilar, Dr. Lynn Goss-Schrag, Dr. Raimund Fromme, Dr. Petra Fromme
Arizona State University, Tempe, AZ, USA

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440 Analysis of Human Serum Albumin Metal Complexes

Vanessa A Bijak1, Michal Gucwa1,2, Michal Szczygiel1,2, Katarzyna Handing1,3, Wladek Minor1
1University of Virginia, Charlottesville, VA, USA. 2Jagiellonian University, Cracow, -, Poland. 3Tango Therapeutics, Boston, MA, USA

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247 Filament formation drives catalysis of glutaminase

Shi Feng, Cody Aplin, Thuy-Tien T. Nguyen, Richard A. Cerione
Cornell University, Ithaca, NY, USA

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55 Efficient tagging of endogenous proteins in human cell lines for structural studies by single particle cryo-EM

Ph.D Wooyoung Choi, Ph.D. Hao Wu, Ph.D. Klaus Yserentant, Ph.D. Bo Huang, Ph.D. Yifan Cheng
UCSF, San Francisco, CA, USA

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392 Cryo-EM uncovers how lysophosphatidic acid (LPA) cooperatively and allosterically activates the inflammatory pain receptor Transient Receptor Potential Vanilloid 1 (TRPV1)
Dr. William R. Arnold, Prof. Yifan Cheng, Prof. David Julius
University of California San Francisco, San Francisco, CA, USA

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431 Macrocycle Refinement: Bambusuril Structures
Dr. Nobuyuki Yamamoto1, Andrew H Olsson1, Elizabeth A Kambas1, Dr. Katherine L VanDenburgh1, Dr. Bo W Laursen2, Dr. Amar H Flood1
1Indiana University, Bloomington, Bloomington, IN, USA. 2University of Copenhagen, Copenhagen, Hovedstaden, Denmark

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226 Magnetic Structure Analysis of NiPS3-xSex
Mr Mario Lopez, Dr Ryan Stadel, Dr Efrain E Rodriguez
University of Maryland, College Park, College Park, MD, USA

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124 Crystal structure of human interleukin-2 in complex with TCB2, a new antibody-drung candidate with antitumor activity
Jieun Kim
POSTECH, Pohang, Gyungbuk, Korea, Republic of

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74 Structural Insights into Dibrominated 2,3-Benzaldehyde Compounds with potential as Antioxidant Agents in Biodiesel
Igor D. Borges1, Antônio S.N. Aguiar1, Leonardo R. Almeida1, Gerardo Aguirre2, Hamilton B. Napolitano1
1Grupo de Química Teórica e Estrutural de Anápolis Universidade Estadual de Goiás, Anápolis, GO, Brazil. 2Instituto Tecnológico de Tijuana, Centro de Graduados e Investigación en Química, Tijuana, BC, Mexico

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471 Investigating near movement-free imaging without GOLD
Md Rejaul Hoq, Min Su
University of Missouri, Columbia, MO, USA

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356 Mode of Substrate Binding for Ketohexokinase across Isozymes and Species Implies an Induced-Fit mechanism
Miss So Young Bae, Professor of Biology Karen N Allen, Professor of Biology Dean R. Tolan
Boston University, Boston, MA, USA

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438 Visualizing Plasmodium falciparum Ultrastructure at Subnanometer Resolution Across the Asexual Blood Stages using in situ cryoET
Wenjing Cheng1, Leonie Anton1, Meseret Haile1, David Cobb2, Chi-Min Ho1
1Columbia University, New York, NY, USA. 2Columbia University*, New York, NY, USA

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424 A serial crystallography error model robust to outlier observations
David W Mittan-Moreau, Vanessa Oklejas, Daniel W Paley, Nicholas K Sauter, Aaron S Brewster

Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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258 Real-Time Data Analysis and Experimental Adjustments with Interceptor at SSRL

Dr. Artem Y Lyubimov
SSRL, Menlo Park, CA, USA

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218 SMALL ANGLE X-RAY SCATTERING APPLICATIONS IN STRUCTURAL BIOLOGY

Dr Lixin Fan1,2, Dr Yun-Xing Wang3,2
1Basic Science Program, Frederick National Laboratory for Cancer Research, Frederick, MD, USA. 2Small Angell X-ray Scattering Facility, National Cancer Institute, Frederick, MD, USA. 3Protein-Nucleic Acid Interaction Section, Center for Structural Biology, Center for Cancer Research, National Cancer Institute, Frederick, MD, USA

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391 Crystal structure of Escherichia coli thiamine pyrophosphate-sensing riboswitch in the apo state

Jason R Stagno1, Hyun Kyung Lee1, Yun-Tzai Lee1, Lixin Fan1, Haley M Wilt1, Chelsie Conrad1, Ping Yu1, Jinwei Zhang2, Genbin Shi1, Xinhua Ji1, Yun-Xing Wang1
1National Cancer Institute, Frederick, MD, USA. 2NIDDK, Bethesda, MD, USA

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388 Relion-based Automation Pipeline

Weimin Wu, Yuri Iozzo, Joseph Batchelor, Anna Park
LMR US, Sanofi, Cambridge, MA, USA

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164 Alternate Realities: Searching for the Optimal Supercell Approximate for Incommensurately Modulated Profilin:Actin Crystals

Jeffrey J Lovelace1, Antoine M M Schreurs2, Loes M J Kroon-Batenburg2, Gloria E O Borgstahl1
1Eppley Institute for Research in Cancer and Allied Diseases, Omaha, NE, USA. 2Bijvoet Center for Biomolecular Research, Faculty of Science, Utrecht University, Utrecht, Utrecht, Netherlands

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165 Growing the PDB Core Archive Using ORCiD Login for Depositing 3D Biostructures with OneDep

Gregg V Crichlow1, Zukang Feng1, Yuhe Liang1, Ezra Peisach1, Irina Persikova1, Jasmine Y Young1, wwPDB Team wwPDB Team1,2,3,4,5,6, Stephen K Burley1,6
1RCSB Protein Data Bank, Rutgers, The State University of New Jersey, Piscataway, New Jersey, USA. 2PDBe, EMBL-European Bioinformatics Institute, Hinxton, England, United Kingdom. 3PDBj, Institute for Protein Research, Osaka University, Osaka, Osaka, Japan. 4EMDB, EMBL-European Bioinformatics Institute, Hinxton, England, United Kingdom. 5BMRB, UConn Health, University of Connecticut, Farmington, Connecticut, USA. 6RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, San Diego, California, USA

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290 Capturing critical sites in disorder-to-order complexation to manipulate protein-protein interfaces

Christina R Bourne, Kevin J Snead
University of Oklahoma, Norman, OK, USA

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347 Single Selenium Atom to Control Nucleic Acid Conformation and Large Crystal Growth
Professor Zhen Huang, Doctor Cen Chen, Doctor Ziyuan Fang, Student Susanna Huang, Student Selina Huang
SeNA Research Institute, Atlanta, GA, USA

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348 Selenium Nucleic Acids for Innovative Structural Biology
Professor Zhen Huang, Doctor Ziyuan Fang, Student Susanna Huang
SeNA Research Institute, Atlanta, GA, USA

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469 Structural basis of DNA binding by the NAC transcription factor ORE1, a master regulator of plant senescence

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478 Structural basis for Cas9-mediated DNA interrogation and editing with 5' truncated sgRNAs.
Kaitlyn A. Kiernan, Jieun Kwon, Melissa Munoz, Bradley Merrill, Miljan Simonovic
University of Illinois, Chicago, IL, USA

YSIG Mixer

Date: Saturday, July 8
Start: 8:00 PM
Room: James Joyce Bar & Restaurant (616 President Street, Baltimore, MD 21202)

The YSIG Mixer aims to provide a relaxed and inclusive environment for early career professionals to meet and mingle with fellow attendees from various backgrounds and industries. Whether you're a recent graduate, a young professional, or transitioning into a new field, this event will offer a valuable platform to foster connections and build meaningful relationships.

Sunday, July 9, 2023

2.1.1: Cool Structures I

8:30 - 11:30am Sunday, 9th July, 2023
Locations Waterview AB
Kamran Ghiassi, Nate Barker, Jeff Bacon, Alex Erickson

This session aims to highlight exciting structures in the realm of chemical crystallography. Examples of 'cool' structures would include small molecules of interest for their chemical or crystallographic properties, structure-property relationships, extended structures, supramolecular materials, and co-crystals. The session will bring the science enabled by chemical crystallographic analysis to the foreground. Speakers will be selected from contributed abstracts. Submissions from students are encouraged

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8:30 - 9:00am
58 Redox-Coupled Structural Distortions in Quasi-1-Dimensional Au2MP2 (M=Tl, Pb, and Bi)
Scott B Lee1, Joseph W Stiles1, Dr. Fang Yuan1, Stephanie R Dulovic1, Dr. Tieyan Chang2,3, Dr. Yu-Sheng Chen2,3, Dr. Leslie M Schoop1
1Princeton University, Princeton, NJ, USA. 2University of Chicago, Chicago, IL, USA. 3Argonne National Laboratory, Lemont, IL, USA

9:00 - 9:30am
88 Catena structures formed by Li(+) with the TCNQF4(-) radical anion or with dianionic, diamagnetic TCNQF4(2-): Comparison to Cu(I)(TCNQX4) compounds (X = H, F, Cl)
Larry R Falvello1, Slavomira Šterbinská1, Milagros Tomás2
1Instituto de Nanociencia y Materiales de Aragón (INMA) and Departamento de Química Inorgánica, CSIC-Universidad de Zaragoza, Zaragoza, Zaragoza, Spain. 2Instituto de Síntesis Química y Catálisis Homogénea (ISQCH) and Departamento de Química Inorgánica, CSIC-Universidad de Zaragoza, Zaragoza, Zaragoza, Spain

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9:30 - 10:00am
37 Novel Manganese-Halide 2-D, 1-D and 0-D Frameworks and their Emission Properties
Michael Onyemuche Ozide, RayVen Gonzales, Dr Tatiana Timofeeva, Dr Raul Luis Castaneda
New Mexico Highlands University, Las Vegas, New Mexico, USA

10:30 - 11:00am
145 Ruthenium crystallography for the connoisseur: a molecular rearrangement, spontaneous resolution, and a disappearing polymorph
Dr. Kamran Ghiassi
Air Force Research Laboratory, Edwards AFB, CA, USA

11:00 - 11:30am
248 High Pressure C60S8: A Well-Travelled Cool Structure

Dr Christine M Beavers1, Dr. Earl F. O'Bannon2, Dr. Kamran B Ghiassi3, Prof Alan L Balch4, Prof Marilyn M Olmstead4
1Rigaku Americas, The Woodlands, Texas, USA. 2Lawrence Livermore National Lab, Livermore, CA, USA. 3Air Force Reseach Laboratory, Edwards AFB, CA, USA. 4University of California, Davis, Davis, CA, USA

2.1.2: Structures from Artificial Intelligence

8:30 - 11:30am Sunday, 9th July, 2023
Locations Laurel CD
Jennifer Wierman, Melanie Vollmar

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

8:30 - 9:00am
175 Use AlphaFold2 at SER-CAT for Crystallographic Analyses and Function Research
Dr. Zheng-Qing Fu1,2, Dr. Zhongmin Jin1,2, Dr. John Chrzas1,2, Michael Molitsky1,2, Dr. James Fait1,2, Prof. John Rose1,2, Prof. Bi-Cheng Wang1,2
1University of Georgia, Athens, GA, USA. 2SER-CAT, APS, Argonne National Lab, Argonne, IL, USA

9:00 - 9:30am
174 CheckMyBlob - Machine learning-based tool for ligand recognition and validation
Joanna Lenkiewicz1, Dariusz Brzezinski1,2, Wladek Minor1
1University of Virginia, Charlottesville, Virginia, USA. 2Poznan University of Technology, Poznan, Wielkopolska, Poland

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9:30 - 10:00am
210 Sweet Protein Crystallography in Post-AlphaFold Era
Tae-Sung YOON
KRIBB, Yuseong-Gu, Daejeon, Korea, Republic of

10:30 - 10:50am
328 Nothing beats good data - Lessons learned from Native-SAD data collection can give the best crystal structure from AlphaFold Molecular Replacement models.
Dr. John P Rose, Dr. Dayong Zhou, Dr. Lirong Chen, Dr. Bi-Cheng Wang

University of Georgia, Athens, GA, USA

10:50 - 11:10am
56 Towards the Structural Analysis of an F-plasmid protein, TraW
Christina Rodriguez, Dr Gerald Audette
York Univeristy, Toronto, ON, Canada

11:10 - 11:30am
241 Monomer and dimer structures of cytochrome bo3 ubiquinol oxidase from Escherichia coli.
Dr. Yirui Guo1,2, Dr. Elina Karimullina3,4, Tabitha Emde1,4, Dr. Zbyszek Otwinowski1, Dr. Dominika Borek1,4, Dr. Alexei Savchenko3,4,5
1University of Texas Southwestern Medical Center, Dallas, TX, USA. 2Ligo Analytics, Dallas, TX, USA. 3University of Calgary, Calgary, Alberta, Canada. 4Centers for Research on Structural Biology of Infectious Diseases (CSBID), Chicago, Illinois, USA. 5University of Toronto, Toronto, Ontario, Canada

2.1.3: New developments in cryoEM and cryoET

8:30 - 11:30am Sunday, 9th July, 2023
Locations Essex A-C
Anchi Cheng, Anthony Fitzpatrick

Technological developments in cryo-EM and cryo-ET have been the driving force moving the field forward. This season will focus on the latest technological developments in cryo-EM, including both hardware and software.

8:30 - 8:50am
308 Enabling automated Cryo-EM data acquisition with Smart EPU
Edward Pryor1, Fanis Grollios2, Bart van Knippenberg2, Yuchen Deng2, Holger Kohr2
1Thermo Fisher Scientific, Hillsboro, OR, USA. 2Thermo Fisher Scientific, Eindhoven, NL, Netherlands

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8:50 - 9:10am
170 High-resolution structure determination at 100kV enabled by new Falcon-C direct electron detector
Adrian Koh, Wen Yang, Dimple Karia, Lingbo Yu, Jeffrey Lengyel, Abhay Kotecha
Thermo Fisher Scientific, Eindhoven, North Brabant, Netherlands

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9:10 - 9:35am
229 Quantifying organellar ultrastructure in cryo-electron tomography using a surface morphometrics pipeline
Dr. Danielle A Grotjahn, Dr. Benjamin A Barad, Michaela Medina, Daniel Fuentes, Dr. R Luke Wiseman
Scripps Research, La Jolla, CA, USA

9:35 - 10:00am
249 A Modular Covalent Labeling System for Ground-Truth Localization of Synaptic Proteins by Cryo-electron Tomography
Richard Held1,2, Maia Azubel2, Jiahao Liang2, Axel Brunger1,2
1Howard Hughes Medical Institute, Chevy Chase, MD, USA. 2Stanford University, Stanford, CA, USA

10:30 - 10:50am
90 High Throughput for High-resolution Cryo Electron Tomography
Shawn Zheng1,2, Yifan Cheng1,2, David Agard1
1University of California San Francisco, San Francisco, CA, USA. 2Howard Hughes Medical Institution, San Francisco, CA, USA

10:50 - 11:10am
310 CryoEM single particle reconstruction with a complex-valued particle stack
Dr. Zbyszek Otwinowski1, Dr. Raquel Bromberg1,2, Dr. Yirui Guo2, Dr. Dominika Borek1
1UT Southwestern Medical Center, Dallas, TX, USA. 2Ligo Analytics, Inc., Dallas, TX, USA

11:10 - 11:30am
183 Outstanding Challenges for Conformational Heterogeneity Analysis in Single-Particle Cryo-EM
Dr Sonya M Hanson
Flatiron Institute, New York, New York, USA

2.1.4: Automation in software, hardware and data processing

8:30 - 11:30am Sunday, 9th July, 2023
Locations Laurel AB
Peter Beaucage, Ruipeng Li

Recent advances such as fourth-generation synchrotron sources, high-flux neutron sources, and fast pixel-array detectors have shifted the primary time-intensive step of SAS and XPCS measurement from data collection to sample delivery and data processing, reduction, and analysis. The experiment lifecycle from measurement to actionable insight has dramatically shortened from weeks of manual data analysis to live, on-the-fly reduction and analysis that enables users to make decisions about next measurement steps 'live' and lays the groundwork for closed-loop autonomous scattering experiments. This session will highlight recent and upcoming advances in the area of high-throughput, automated, and autonomous data processing. While beamlines and facilities will be a major focus, examples of laboratory source automation and user-developed data pipelines are also encouraged.

8:30 - 9:00am
30 PyHyperScattering: a collaborative framework for highly multidimensional scattering dataset loading, reduction, analysis, and display
Dr Peter A Beaucage
NIST Center for Neutron Research, Gaithersburg, MD, USA

9:00 - 9:30am
101 A Tool for Automating the Repetitive Part of PXRD User Reports
Dr. Matthew L. Brown
University Of British Columbia, Kelowna, BC, Canada

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9:30 - 10:00am
322 Analysis pipeline for in-situ SAXS/WAXS experiments
Ruipeng Li
NSLS II, Brookhaven National Lab, Upton, NY, USA

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10:30 - 11:00am
264 Robotic sample preparation and delivery for autonomous material discovery at APS-U 8-ID Beamlines
Dr. Qingteng Zhang
Argonne National Laboratory, Lemont, IL, USA

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11:00 - 11:30am
244 Automation for data collection, processing, and analysis at the LiX beamline
Lin Yang
Brookhaven National Laboratory, Upton, NY, USA

2.1.5: DEI: expanding access & opportunities in structural science

8:30 - 11:30am Sunday, 9th July, 2023
Locations Kent A-C
Eta Isiorho, Christina Bourne
DEI: expanding access & opportunities in structural science

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8:30 - 9:00am
332 Increasing STEM Persistence Through CUREs and Community
Krystle J McLaughlin
Vassar College, Poughkeepsie, NY, USA

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9:00 - 9:30am
331 Developing Training and Educational Resources in Biomolecular Structural Biology for Diverse Audiences
Dr. Shuchismita Dutta
RCSB Protein Data Bank and Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, NJ, USA

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9:30 - 10:00am
315 A Snowball Effect of Opening Doors and Offering Sustained Support for Early Career Scientists
Dr. Lindsey R. F. Backman
Whitehead Institute for Biomedical Research, Cambridge, MA, USA

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10:30 - 10:50am
113 Integration of structural science to broaden the participation of diverse learners in STEM
Dr. Oluwatoyin A Asojo
Hampton University, Hampton, VA, USA

10:50 - 11:10am
350 Crystallizing Student-Interest in Biochemistry
Susanna Huang1,2, Selina Huang1
1SeNA Research Institute, Atlanta, GA, USA. 2Georgia Institute of Technology, Atlanta, GA, USA

PL1: Etter Award

11:30am - 12:30pm Sunday, 9th July, 2023
Locations Essex A-C

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65 The dynamic side of crystals: How structure influences function in the solid-state
Kristin M Hutchins
Texas Tech University, Lubbock, TX, USA

2.2.1: Cool Structures II

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Waterview AB
Nate Barker, Jeff Bacon, Alex Erickson, Kamran Ghiassi

2:00 - 2:30pm
11 Structural basis of DNA binding by the NAC transcription factor ORE1, a master regulator of plant senescence
Inseop Chun1, Hyo Jung Kim2, Sunghyun Hong3, Yeon-Gil Kim4, Min-Sung Kim5
1Postech, pohang-si, Gyeongbuk, Korea, Republic of. 2center for plant aging Research, Institute for Basic Science, Daegu, Gyeongbuk, Korea, Republic of. 3center for genome Engineering, institute for Basic Science, Daejeon, Chungbuk, Korea, Republic of. 4Pohang Accelerator Lab, POSTECH, Pohang, Gyeongbuk, Korea, Republic of. 5Postech, Pohang, Gyeongbuk, Korea, Republic of

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2:30 - 3:00pm
20 Characterization of a putative periplasmic cystine binding protein from Candidatus Liberibacter asiaticus
Prof Ashwani Kumar Sharma1, Dr. Pranav Kumar1, Dr. Pooja Kesari1, Mr. Sunil Kokane2, Dr. Dilip K Ghosh2, Prof. Pravindra Kumar1
1IIT Roorkee, Roorkee, Uttarakhand, India. 2ICAR-CCRI, Nagpur, Maharashtra, India

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3:30 - 4:00pm
284 A metal dependent conformational change provides a structural basis for the inhibition of E. Coli CTP synthase by gemcitabine-5'-triphosphate

Dr Matthew J Mcleod1, Norman Tran2, Dr Gregory D McCluskey3, Tom D Gillis3, Prof Stephen L Bearne3, Prof Todd Holyoak2
1Cornell University, Ithaca, NY, USA. 2University of Waterloo, Waterloo, ON, Canada. 3Dalhousie University, Halifax, NS, Canada

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4:00 - 4:30pm
261 Influence of Hydrogen bonding on the Formation of 0D or 1D Manganese-Halide Hybrid Materials
Kandee Gallegos, Michael Ozide, Dr. Raúl Castañeda
New Mexico Highlands University, Las Vegas, NM, USA

4:30 - 5:00pm
17 Think, Pair, Share: Insight into Electronic Structure from Single Crystal Structures of Redox-Active Ligands
Sophie W Anferov, Lauren E McNamara, Dr Alexander S Filatov, Professor John S Anderson
University of Chicago, Chicago, Illinois, USA

2.2.2: Artificial Intelligence, Machine Learning, and Other Data Science Techniques Applied to Structure Determination, materials characterization, experiment control and data analysis

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Laurel CD
Taylor Sparks, William Ratcliff

In this session, we will have an exciting range of talks on applications of data science, machine learning, and artificial intelligence towards structure determination. Topics covered will include advances in automation of experiments, adaptive design, structural modeling, generative models, and structural prediction.

2:00 - 2:30pm
86 Machine Learning-Driven Automated Scanning Probe Microscopy
Yongtao Liu1, Rama Vasudevan1, Kyle Kelley1, Maxim Ziatdinov1, Sergei Kalinin2
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2University of Tennessee, Knoxville, TN, USA

2:30 - 3:00pm
132 Machine learning assisted automation of single crystal neutron diffraction
Yiqing Hao, Erxi Feng, Dan Lu, Leah Zimmer, Zachary Morgan, Bryan C. Chakoumakos, Guannan Zhang, Huibo Cao
Oak Ridge National Laboratory, Oak Ridge, TN, USA

3:30 - 3:50pm
108 Semi and Self Supervised approaches to Space Group and Bravais Lattice Determination
Dr. William D Ratcliff

NIST, Gaithersburg, Maryland, USA

3:50 - 4:10pm
72 How to Identify Nonlinear Optical Crystals for THz Generation
Sin Hang (Enoch) Ho1, Gabriel A. Valdivia-Berroeta2, Zachary B. Zaccardi1, Sydney K. F. Pettit1, Bruce Wayne Palmer1, Matthew J. Lutz1, Claire Rader1, Brittan P. Hunter1, Natalie K. Green1, Connor Barlow1, Coriantumr Z. Wayment1, Daisy J. Harmon1, Paige Petersen1, Dr. Stacey J. Smith1, Dr. David J. Michaelis1, Jeremy A. Johnson1
1Brigham Young University, Provo, Utah, USA. 2Boehringer Ingelheim Inc., Connecticut, Connecticut, USA

4:10 - 4:30pm
46 Refinement of crystal structures at ultralow resolution with assistance from AlphaFold modeling and Rosetta optimization
Wei Wang, Wayne A Hendrickson
Columbia University, New York, NY, USA

4:30 - 4:50pm
143 Growth of the PDB Archive Requires Transition to PDBx/mmCIF Format Files
Sutapa Ghosh1, Zukang Feng1, Yuhe Liang1, Ezra Peisach1, Irina Persikova1, Chenghua Shao1, Jasmine Y Young1, wwPDB Team1,2,3,4,5, Stephen K Burley1,6
1RCSB Protein Data Bank, Rutgers, The State University of New Jersey, Piscataway, NJ, USA. 2PDBe, EMBL-European Bioinformatics Institute, Hinxton, Cambridgeshire, United Kingdom. 3PDBj, Institute for Protein Research, Osaka University, Osaka, Osaka, Japan. 4EMDB, EMBL-European Bioinformatics Institute, Hinxton, Cambridgeshire, United Kingdom. 5BMRB, UConn Health, Farmington, CT, USA. 6RCSB Protein Data Bank, San Diego Supercomputer Center, University of California San Diego, La Jolla, CA, USA

2.2.3: General Interest II

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Waterview CD
Tim Stachowski, Victoria Drago

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

2:00 - 2:20pm
283 High Pressure X-ray Diffraction for Visualization of Transient Intermediates in the Tryptophan Synthase Mechanism
Laurel B Leber1, Victoria N Drago2, D Marian Szebenyi3, Robert S Phillips4, Timothy C Mueser1
1Department of Chemistry and Biochemistry, University of Toledo, Toledo, OH, USA. 2Oak Ridge National Laboratory, Oak Ridge, TN, USA. 3Cornell High Energy Synchrotron Source, Ithaca, NY, USA. 4Department of Chemistry, University of Georgia, Athens, GA, USA

2:20 - 2:40pm
313 The Importance of the Water Network within the Leukotriene A4 Hydrolase Binding Site for Aminopeptidase Activators
Kyung Hyeon Lee1,2, Soo Hyeon Lee2, Jiangdong Xiang3, Greg Petruncio1, Yun M Shim4, Mikell Paige1, Schroeder M Noble2
1George Mason University, Manassas, VA, USA. 2Walter Reed Army Institute of Research, Silver Spring, MD, USA. 3Shanghai General Hospital, Shanghai, Shanghai, China. 4University of Virginia, Charlottesville, VA, USA

2:40 - 3:00pm
69 Comparing ATAD2/B bromodomain structure-function differences in the dynamic epigenetic landscape
Margaret Phillips1, Isabelle A. Kressy1, Brian Boyle1, Jay C. Nix2, Karen C. Glass1
1University of Vermont, Burlington, VT, USA. 2Molecular Biology Consortium, Berkeley, CA, USA

3:30 - 4:00pm
224 Role of Receptor Binding Domain Conformation on Spillover Potential of Cambodian Sarbecovirus
Samantha K. Zepeda1, Tyler N. Starr2,3,4, Allison J. Greaney2,5, Andrew Muenks1,6, Alexandra C. Walls1,3, Young-Jun Park1, Davide Corti7, Frank DiMaio1,6, Jesse D. Bloom2,3,5, David Veesler1,3
1Department of Biochemistry, University of Washington, Seattle, WA, USA. 2Basic Sciences Division, Fred Hutchinson Cancer Research Center, Seattle, WA, USA. 3Howard Hughes Medical Institute, Seattle, WA, USA. 4University of Utah, Salt Lake City, UT, USA. 5Department of Genome Sciences, University of Washington, Seattle, WA, USA. 6Institute for Protein Design, University of Washington, Seattle, WA, USA. 7Humabs BioMed SA, Bellinzona, -, Switzerland

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4:00 - 4:30pm
188 Structural insights into N-linked glycan remodeling of the SARS-CoV-2 spike protein
Suruchi Singh1, Yi Liu2, Meghan Burke2, Benjamin Jennings3, Debajit Dey1, Balraj Doray3, Stephen Stein2, S. Saif Hasan1
1Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, Baltimore, MD, USA. 2Mass Spectrometry Data Center, Biomolecular Measurement Division, National Institute of Standards and Technology, Gaithersburg, MD, USA. 3Department of Internal Medicine, Hematology Division, Washington University School of Medicine, St. Louis, MO, USA

4:30 - 5:00pm
163 GPCR Affecting Fatty Acid Amide produced by Non-Ribosomal Peptide Synthetase Cluster
Jitendra Singh, Dr Sarah Chamberlain, Professor Thomas D Grant, Professor Andrew M Gulick
Jacobs School of Medicine and Biomedical Sciences, University at Buffalo, Buffalo, NY, USA

2.2.4: Machine learning in cryo-EM

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Essex A-C

Alexis Rohou, Michael Cianfrocco

Machine learning has been increasingly applied in all aspects of cryo-EM, particularly in cryo-EM image processing. This session will focus on algorithm development and the application of machine learning in cryo-EM. We will highlight how machine learning affects the cryo-EM structure determination process, including data collection, micrograph and tomogram interpretation, 3D structure analysis, model building, and annotation.

2:00 - 2:30pm
294 Using Machine Learning for Regularization in Cryo-EM
Dimitry Tegunov
Genentech, South San Francisco, CA, USA

2:30 - 3:00pm
334 Deep learning for reconstructing in situ structural landscapes from cryo-electron tomography
Prof. Ellen D Zhong
Princeton University, Princeton, NJ, USA

3:30 - 3:50pm
62 CryoFAST™: Automated Cryo-Electron Microscopy Data Acquisition using Machine Learning
Mr Elliot Gray1, Dr Dmitry Lyumkis2, Dr Atousa Mehrani2, Mr Narasimha Kumar1
1HTI Inc, Portland, Oregon, USA. 2Salk Institute, La Jolla, California, USA

3:50 - 4:10pm
301 3D Flexible Refinement: Determining Structure and Motion of Flexible Proteins from Cryo-EM
Ali Punjani1,2, Dr. David Fleet2
1Structura Biotechnology Inc., Toronto, ON, Canada. 2University of Toronto, Toronto, ON, Canada

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4:10 - 4:30pm
75 Quality Assessment and Biomolecular Structure Modeling for Cryo-EM using Deep Learning
Genki Terashi, Xiao Wang, Tsukasa Nakamura, Devashish Krishna Prasad, Daisuke Kihara
Purdue University, West Lafayette, Indiana, USA

2.2.5: Serial Crystallography

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Kent A-C
Iris Young, Preta Fromme

Alongside rotation crystallography, serial crystallography has emerged as a powerful method for structure determination, with advantages for certain samples or experimental designs. At XFELs, so-called "diffraction-before-destruction" enables probing extremely radiation sensitive materials, from metalloenzymes to MOFs. Serial crystallography also opens up time-resolved experiments across time scales ranging from seconds to femtoseconds. Such experiments place new demands on sample delivery, instrumentation, and data processing methods as well. Finally, the introduction of microED as a robust

structure determination technique raises the possibility of serial electron diffraction as an analogous technique to serial X-ray diffraction. This session highlights some of these advances, their unique promises and challenges, and their context at the forefront of crystallographic structure solution.

2:00 - 2:20pm
335 High-resolution Crystal Structures of Transient Intermediates in the Phytochrome Photocycle
Emina A Stojkovic1, Tek Narsingh Malla2, Luis Aldama1, Suraj Pandey2, Melissa Carrillo1, Sebastian Westenhoff3, Marius Schmidt2
1Northeastern Illinois University, Chicago, IL, USA. 2University of Wisconsin - Milwaukee, Milwaukee, WI, USA. 3University of Gothenburg, Gothenburg, Goteborg, Sweden

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2:20 - 2:40pm
305 Hot and Bothered: Perturbing protein dynamics with temperature-jump for time-resolved crystallography experiments
Prof. Michael C Thompson
University of California, Merced, Merced, CA, USA

2:40 - 3:00pm
126 Watching the release of a photopharmacological drug from its target using time-resolved serial crystallography
Dr. Tobias Weinert, Dr. Maximilian Wranik, Prof. Dr. Michel O Steinmetz, Dr. Jörg Standfuss
Paul Scherrer Institute, Villigen PSI, Aargau, Switzerland

3:30 - 3:50pm
106 Current status of serial crystallography at SPring-8 MX beamlines
Kunio Hirata1, Hiroaki Matsuura1, Yoshiaki Kawano1, Naoki Sakai2, Kazuya Hasegawa2, Takashi Kumasaka2, Masaki Yamamoto1
1RIKEN/SPring-8 Center, Sayo-gun, Hyogo, Japan. 2JASRI/SPring-8, Sayo-gun, Hyogo, Japan

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3:50 - 4:10pm
236 Micro-structured polymer fixed-targets (MISP-chips) for serial crystallography at synchrotrons and XFELs
Melissa Carrillo, Thomas James Mason, John Henry Beale, Celestino Padeste
Paul Scherrer Institute, Villigen, Aargau, Switzerland

4:10 - 4:30pm
366 XRAI: Simulation informed neural networks for guiding crystallography experiments
Derek Mendez1, Artem Lyubimov1, Jinhu Song1, Scott McPhillips1, Mike Soltis1, James M Holton2,1,3, Aina E Cohen1
1SLAC, Menlo Park, CA, USA. 2LBNL, Berkeley, CA, USA. 3UCSF, San Francisco, CA, USA

4:30 - 4:50pm
349 Improving Data Collection Efficiency in small-molecule Serial Femtosecond Crystallography at X-ray Free Electron Lasers

Ms. Elyse A Schriber1, Dr. Daniel Paley2, Dr. Raymond Sierra3, Dr. Aaron Brewster2, Prof. James N. Hohman4
1Institute of Materials Science, University of Connecticut, Storrs, CT, USA. 2Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 3Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA. 4Department of Chemistry, University of Connecticut, Storrs, CT, USA

2.2.6: Enzyme allostery

2:00 - 5:00pm Sunday, 9th July, 2023
Locations Laurel AB
Will Thomas, Max Watkins

Proper regulation is fundamental to biological systems, and this regulation often proceeds through allosteric control and binding of effectors at sites other than an active site. While not quite the “spooky action at a distance” that Einstein warned of, the communication of allosteric binding is nonetheless quite the curiosity, often involving long intra-protein distances and surprising or intricate changes in protein conformational ensemble. Though still challenging to study, uncovering the mysteries of allostery are of increasing interest for exploring novel avenues of pharmaceutical development as well as for understanding protein dynamics at a fundamental level. Fortunately, recent advances in structural biology techniques, especially solution scattering and cryo-electron microscopy, have increasingly enabled global-level studies of allosterically-driven conformational and oligomeric state changes. This session focuses on the use of structural biology techniques, with a particular emphasis on solution small-angle scattering, to gain insight into mechanisms of allosteric regulation, making them a little less “spooky” but no less wondrous.

2:00 - 2:20pm
327 Cryo-EM reveals the structural origins of asymmetric electron transfer in nitrogenase-like enzymes
Dr Rajnandani Kashyap, Dr Jaigeeth Deveryshetty, Dr Edwin Antony
Saint Louis Univerity, St. Louis, Missouri, USA

2:20 - 2:40pm
51 Solution characterization of the dynamic conjugative entry exclusion protein TraG
Nicholas J Bragagnolo, Dr. Gerald F Audette
York University, Toronto, Ontario, Canada

2:40 - 3:00pm
82 Molecular Basis of Acetylated Lysine Recognition by the Plasmodium falciparum Bromodomain Protein 1
Karen C. Glass1, Ajit K. Singh1, Mirabella P. Vulikh1,2, Margaret Phillips1, Marco Tonelli3, Kiera L. Malone1, Saleh Alkrimi2, Jay C. Nix4
1University of Vermont College of Medicine, Burlington, VT, USA. 2Albany College of Pharmacy and Health Sciences, Colchester, VT, USA. 3University of Wisconsin-Madison, Madison, WI, USA. 4Advanced Light Source, Berkeley, CA, USA

3:30 - 4:00pm
130 Structural Intermediates of Phenylalanine Hydroxylase Revealed by Disruption of a Key Intramolecular Interaction
Kushol Gupta1, Yara Mustafa1, Melanie Reuter2,1, Emilia Arturo3,4, George Merkel4, Eileen Jaffe4
1Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA. 2Temple University, Philadelphia, PA, USA. 3Department of Biochemistry and Molecular Biology, Drexel University College of Medicine, Philadelphia, Philadelphia, PA, USA. 4Molecular Therapeutics Program, Fox Chase Cancer Center, Philadelphia, PA, USA

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4:00 - 4:30pm
43 RESOLVING PHOSPHOLIPASE C REGULATION
Dr. Isaac J Fisher1, Dr Kaushik Muralidharan2, Kennedy Outlaw1, Elisabeth Garland-Kuntz1
1Purdue University, West Lafayette, IN, USA. 2Nationwide Children's Hospital, Cincinnati, OH, USA

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4:30 - 5:00pm
197 Turning Ribonucleotide Reductase On and Off
Gisele A Andree, Andrew J Dorfeuille, Michael A Funk, Gyunghoon Kang, Talya S Levitz, Kelsey R Miller, Gerardo Perez Goncalves, Dana E Westmoreland, Christina M Zimanyi, Catherine L Drennan
MIT, Cambridge, MA, USA

Poster Session #2

5:30 - 7:30pm Sunday, 9th July, 2023
Locations Exhibit Hall

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429 Structural studies of the human particulate guanylyl cyclase receptor A (pGC-A), to support therapeutics for cardiovascular diseases.
Mr Kohilan Jeyasothy1,2, Dr Shangji Zhang1, Dr Jose M. Martin-Garcia1, Dr Domingo M. Aguilar1, Dr Debra T Hansen1, Dr Petra Fromme1,2, Dr John C. Burnett Jr3
1Arizona State University, Biodesign Center for Applied Structural Discovery, Tempe, Arizona, USA. 2Arizona State University, School of Molecular Sciences, Tempe, Arizona, USA. 3Mayo Clinic, Rochester, Minnesota, USA

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415 Biophysical Characterization of the Pseudomonas aeruginosa BqsR/BqsS Two-Component System
Alexander Paredes1, Dr. Janae Baptiste-Brown2, Chioma Iheacho1, Dr. Aaron T Smith1
1University of Maryland Baltimore County, Baltimore, MD, USA. 2Spelman College, Atlanta, GA, USA

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409 Determining the Crystal Structure of Collagenase H S1 Domain and Developing a SAXS-Derived Enveloped Structure of its Binding Domains-Minicollagen Complex
Adjoa O. Bonsu1, Dr. Takehiko Mima2, Dr. Osamu Matsushita2, Dr. Joshua Sakon1
1Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, USA. 2Department of Bacteriology, Okayama University Graduate School of Medicine, Tsushima-Naka, Okayama, Japan

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359 Structural Studies of Non-structural protein 15 (Nsp15) Endoribonuclease from Original SARS-CoV-2 and its Variant Epsilon for Therapeutic Intervention
Manashi Sonowal, Nirupa Nagaratnam, Dhenugen Logeswaran, Rebecca Jernigen, Raimund Fromme, Petra Fromme
Arizona State University, Tempe, Arizona, USA

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441 The use of CheckMyMetal for modeling metal binding sites in low-resolution protein structures
Michal Gucwa1,2, Joanna Lenkiewicz1, Michal Szczygiel1,2, Aziza Aripova1, Wladek Minor1
1University of Virginia, Charlottesville, Virginia, USA. 2Jagiellonian University, Krakow, Lesser Poland, Poland

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401 The crystal structure of a PTE RNA element from a cactus virus that binds human eIF4E.
Author Manju Ojha1, Deepak Koirala2
1University of Maryland Baltimore County, Baltimore, MD, USA. 2Univeristy of Maryland, Baltimore, MD, USA

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398 Structural studies of domain IV RNA from type I picornaviral internal ribosome entry sites
Hasan Al Banna, Naba Krishna Das, Deepak Koirala
University of Maryland Baltimore County, Baltimore, MD, USA

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396 Structural and biophysical characterization of the Vibrio cholerae ferrous iron transport protein B (FeoB)
Mark A Lee, Dr. Aaron T Smith
University of Maryland, Baltimore County, Baltimore, MD, USA

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386 Structure studies of IMP-specific phosphatase ISN1 from Saccharomyces cerevisiae
sujeong byun, sangkee rhee
Seoul National University, Seoul, Gwanak District, Korea, Republic of

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380 The crystal structure of coxsackievirus 5’ RNA replication platform
Naba K. Das1, Nele M. Hollmann1,2, Deepak Koirala1
1Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, MD, USA. 2Howard Hughes Medical Institute, University of Maryland Baltimore County, Baltimore, MD, USA

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318 Understanding Activation and Inhibition of Leukotriene A4 Hydrolase Aminopeptidase by 4MDM-ARM1 Hybridized Modifiers
Kyung Hyeon Lee1,2, Soo Hyeon Lee2, Jiangdong Xiang3, Greg Petruncio1, Yun M Shim4, Mikell Paige1, Schroeder M Noble2
1George Mason University, Manassas, VA, USA. 2Walter Reed Army Institute of Research, Silver Spring, MD, USA. 3Shanghai General Hospital, Shanghai, Shanghai, China. 4University of Virginia, Charlottesville, VA, USA

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173 Structural basis for anti-cancer activity of a novel metoxiflavona derivative from Strychnos pseudoquina
Dr Marianna C. Silva1, Dr Antônio C.S. C. S. Menezes2, Dr João H. Araujo-Neto3, Dr Hamilton B. Napolitano1,2
1Universidade Evangélica de Goiás, Anápolis, GO, Brazil. 2Universidade Estadual de Goiás, Anápolis, GO, Brazil. 3Universidade de São Paulo, São Carlos, SP, Brazil

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159 Structure of the catalytically active APOBEC3G bound to a DNA oligonucleotide inhibitor reveals tetrahedral geometry of the transition state
Atanu Maiti1, Adam K Hedger2,3, Wazo Myint1, Vanivilasini Balachandran1, Jonathan K Watts4,3, Celia A Schiffer4, Hiroshi Matsuo1
1Cancer Innovation Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MD, USA. 2Institute for Drug Resistance and Department of Biochemistry and Molecular Biotechnology, University of Massachusetts Chan Medical School,, Worcester, MA, USA. 3RNA Therapeutics Institute, University of Massachusetts Chan Medical School, Worcester, MA, USA. 4Institute for Drug Resistance and Department of Biochemistry and Molecular Biotechnology, University of Massachusetts Chan Medical School, Worcester, MA, USA

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73 Synthesis and Characterization of Potentially Catalytic Tolunitrile Adducts of Rhodium(II) Acetate
Malachi O Cope, Dr. Cassandra T Eagle, Alain M Beauparlant
East Tennessee State University, Johnson City, TN, USA

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390 Structural characterization of a metal transporter from Bacillus subtilis
Dia Zheng, Yuri Silva, Oriana S Fisher
Lehigh University, Bethlehem, PA, USA

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384 Exploring the Interplay of Dynamics and Allosteric Regulation in PTP1B
Ammaar A Saeed, Margaret A Klureza, Doeke R Hekstra
Harvard University, Cambridge, MA, USA

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418 Understanding bioterrorism agent Francisella tularensis virulence through CapBCA protein
Madurangi E Ranaweera1, Dr. Rebecca J Jernigan1, Dr. Debra T Hansen1, Dr. Petra Fromme1,2
1Biodesign Center for Applied Structural Discovery, Arizona State University, Tempe, Az, USA. 2School of Molecular Sciences, Arizona State University, Tempe, Az, USA

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167 Interaction between JULGI and G-quadruplex: Prominent factor of strategy for improving crop yield
Eunhye Jung
POSTECH, Pohang, Pohang, Korea, Republic of

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435 Structural Characterization of a Small Molecule-RNA Triple Helix Complex
Madeline M Glennon1, Krishna M Shivakumar1, Martina Zafferani2, Anita Donlic2, Amanda E Hargrove2, Jessica A Brown1
1University of Notre Dame, South Bend, IN, USA. 2Duke University, Durham, NC, USA

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36 A combined structural, spectroscopic, electrochemical, and magnetic study of Nickel(II) pyrazolates: dinuclear [Ni2], linear [Ni3], and triangular [Ni3] incorporating five-/six-coordinate Ni2+ ions.
Zhichun Shi1, Dr Indranil Chakraborty1, Prof Yiannis Sanakis2, Prof Raphael G Raptis1
1Florida International University, Chemistry Department, Miami, FL, USA. 2Institute of Nanoscience and Nanotechnolgy, National Centre of Scientific Research "Demokritos", Aghia Paraskevi, Attiki, Greece

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38 The temperature-dependent activity and structural changes of enzymes revealed using multi-temperature crystallography
Dr. Matthew J McLeod1, Sarah Barwell2, Dr. Todd Holyoak2, Dr. Robert Thorne1
1Cornell, Ithaca, New York, USA. 2University of Waterloo, Waterloo, Ontario, Canada

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428 Microstructural characterization of charged polymers involved in Molecular mechanisms of moisture driven Direct Air Capturing (Mission DAC)
Gayathri Yogaganeshan, Petra Fromme
Arizona State University, Tempe, Arizona, USA

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437 A novel GUI for serial data classification using Machine Learning approaches
Gihan K Ketawala, Professor Petra Fromme, Ast Professor Sabbine Botha
Arizona State University, Tempe, Arizona, USA

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425 Understanding the emergence of CDW order in KCP via a 2D XY model
Dr Arianna Minelli1, Ariana Verme2, Dr Emma Wolpert3, Prof Ella Schmidt4, Dr Feng Ye1, Prof Andrew Goodwin2
1ORNL, Oakridge, Tenneesee, USA. 2University of Oxford, Oxford, Oxfordshire, United Kingdom. 3Imperial College London, London, London, United Kingdom. 4Universität Bremen, Bremen, Germany, Germany

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416 1D-Coordination Polymers and Discrete Complexes With {LnCu5}3+ Metallamacrocycles Demonstrating Single Molecule Magnet Behavior or Magnetocaloric Effect
Anna Pavlishchuk1,2, Matthias Zeller1, Eva Rentschler3, Fabrice Pointillart4, Anthony W. Addison5
1Purdue Universtity, West Lafayette, IN, USA. 2L. V. Pisarzhevskii Institute of Physical Chemistry, Kyiv, Kyiv, Ukraine. 3Johannes Gutenberg University, Mainz, Rhineland-Palatinate, Germany. 4The University of Rennes 1, Rennes, Brittany, France. 5Drexel University, Philadelphia, PA, USA

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417 Understanding the Structure and Properties of the Elusive Non-stoichiometric Lead dioxide
Tiffany L Kinnibrugh1, Tim Fister1, Xiaoping Wang1, David Bazak2, Ajay Karakoti2, Vijayakumar Murugesan2
1Argonne National Laboratory, Lemmont, IL, USA. 2Pacific Northwest National Laboratory, Richland, WA, USA

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407 Cryogenic Electron Microscope Facility at KEK-SBRC

Akihito Ikeda, Masato Kawasaki, Takayuki Kubota, Misato Yamamoto,Yusuke Yamada, Satomi Inaba-Inoue, Akira Takasu, Shinji Aramaki, Chiho Masuda, Naruhiko Adachi, Toshio Moriya, Toshiya Senda
Structural Biology Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tsukuba, Ibaraki, Japan

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400 Structural properties of the valence tautomerism interconversion in Co(diox)2(Py)2 crystals
Ludmila Leroy1,2, Ellen Kiens3, Camila Bacellar4, Majed Chergui5, Carlos Pinheiro1
1Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil. 2Swiss Light Source, Paul Scherrer Institut, Villigen, AR, Switzerland. 3University of Twente, Drienerlolaan, OV, Netherlands. 4SwissFEL, Paul Scherrer, Villigen, AR, Switzerland. 5École Polytechnique Federal de Lausanne, Lausanne, VD, Switzerland

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131 Time-resolved reciprocal space mapping of ferroelectric perovskites under an alternative electric field
Hyeokmin Choe
Bowie State University, Bowie, Maryland, USA

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16 Teaching the Reciprocal Lattice
Carla Slebodnick1, Maureen M. Julian2, Francis T. Julian3
1Department of Chemistry, Virginia Tech, Blacksburg, VA, USA. 2Department of Materials Science and Engineering, Virginia Tech, Blacksburg, VA, USA. 3Oliver Wyman, Princeton, NJ, USA

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355 Recent Developments at the Biological Small-Angle Neutron Scattering Instrument (Bio-SANS) at Oak Ridge National Laboratory
Dr Hugh O'Neill, Dr Sai Venkatesh Pingali, Dr Wellington Leite, Dr Kevin Weiss, Qiu Zhang, Dr. Hong-Hai Zhang, Dr. Luke Heroux, Dr. Volker Urban
Oak Ridge National Laboratory, Oak Ridge, TN, USA

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422 The Prediction, Observation, and Analysis of a New Form of Cannabidiol
Dr Lina Mardiana, Dr Michael J Hall, Prof Michael R Probert
Newcastle University, Newcastle upon Tyne, Tyne and Wear, United Kingdom

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421 Implementing encapsulated nanodroplet crystallisation techniques to crystallise natural products
Dr Michael J Hall1, Dr Alex Longcake1, Prof Michael R Probert1, Prof Nicholas H Oberlies2, Dr Lina Mardiana1
1Newcastle University, Newcastle upon Tyne, Tyne and Wear, United Kingdom. 2The University of North Carolina, Greensboro, North Carolina, USA

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420 Statistically Guided High-Throughput Polymorph Screening of ROY
Jake Weatherston, Dr Michael J Hall, Dr Michael R Probert
Newcastle University, Newcastle upon Tyne, Tyne and Wear, United Kingdom

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394 Effect of Crystal Structure on Photoreactivity of Unsaturated Carboxylic Acids in the Solid State

Mehdi Esmaeili, Dmitriy V Soldatov
University of Guelph, Guelph, Ontario, Canada

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367 Biosynthesis of deuterated lipids for structural and biophysical characterization of biomembranes and membrane proteins
Qiu Zhang1, Honghai Zhang1, Matthew Keller2, Wellington Leite1, Shuo Qian1, Robert Hettich1, Hugh O'Neill1
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2University of Tennessee, Knoxville, Knoxville, TN, USA

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362 CryoFIB milling of large tissue samples with on-the-fly localization
Dr Xueming Li
School of Life Science, Tsinghua University, Beijing, Beijing, China

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467 Micro-electron diffraction applications in the structural analysis of metal-organic frameworks and amorphous phases prepared by mechanochemistry
Dr. SILVINA PAGOLA1, Dr. Johannes Merkelbach2, Dr. Tarek Abdel-Fattah3
1Old Dominion University, Norfolk, VA, USA. 2ELDICO SCIENTIFIC, Villigen, Aargau, Switzerland. 3Christopher Newport University, Newport News, VA, USA

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180 Approximate Symmetry in P2 and C2 Organic Structures
Professor Carolyn P Brock
University of Kentucky, Lexington, KY, USA

2.3.1: Career Odysseys

7:30 - 9:00pm Sunday, 9th July, 2023
Locations Essex A-C
Samantha Powell, Daniel Kneller

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

7:30 - 7:40pm
60 My cryoEM path to Genentech
Alexis Rohou
Genentech, South San Francisco, CA, USA

7:40 - 7:50pm
238 Path to PUI as a Protein Crystallographer
Krystle J McLaughlin
Vassar College, Poughkeepsie, NY, USA

7:50 - 8:00pm

151 Transitioning from Academia to a Cryo-EM CRO
Emily Armbruster
NanoImaging Services, Woburn, MA, USA

8:00 - 8:10pm
49 Career bio for participation as a panelist in the "Career Odysseys" session
Cameron Noland
Merck, South San Francisco, CA, USA

8:10 - 8:20pm
342 From Lab to Leadership: Pursuing Passion and Purpose
Lisa J. Keefe
Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA. IMCA-CAT, Lemont, IL, USA

Monday, July 10, 2023

3.1.1: Total Scattering: Applications and advances in complex materials.

8:30 - 11:30am Monday, 10th July, 2023
Locations Waterview CD
Daniel Olds, Allyson Fry-Petit

This session will feature a mixture of talks on developments in both neutron and x-ray total scattering techniques (e.g. AI-informed modeling and experimental control, multimodal analysis, dynamical PDF, 3D-ΔPDF, in-situ experimental capabilities, thin-film PDF, etc) and applications of total scattering to topical materials. As total scattering methods continue to grow in impact in diverse fields, this session will be useful for newcomers and experienced practitioners alike

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8:30 - 8:50am
123 Exceptionally large magnetovolume effect in MnTe driven by a novel magnetostructural coupling mechanism
Benjamin A. Frandsen
Brigham Young University, Provo, Utah, USA

9:10 - 9:30am
116 Combined atomic pair distribution function and EXAFS analysis of local structural study of MoTe2
Sumit Khadka1, Byron Freelon2, Leighhane Gallington3, Yu-Cheng Shao4, Milinda Abeykoon5
1Texas Center for Superconductivity, Houston, TX, USA. 2University of Houston, Houston, TX, USA. 3Advanced Photon Source (X-ray Science Division), Chicago, IL, USA. 4National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu, Taiwan. 5Brookhaven National Laboratory, Upton, NY, USA

9:30 - 10:00am
263 Investigation of the manipulation and interaction of magnetic and electric dipoles on the pyrochlore lattice
Geneva Laurita1, Owen Bailey1, Jake O'hara1, Daniel Olds2, Hayden Evans3
1Bates College, Lewiston, ME, USA. 2Brookhaven National Lab, Upton, NY, USA. 3NIST, Gaithersburg, MA, USA

10:30 - 10:50am
67 Metal Oxygen Bond Anisotropy and Size Effects Scattering in V1-xMxO2 (M = Nb, Mo)
Jacob F Phillips1, Dr. Top B Rawot Chhetri1, Dr. Matthew A Davenport1, Dr. Tyra C Douglas1, Logan M Whitt1, Dr. Stephan Rosenkranz2, Dr. Raymond Osborn2, Dr. Matthew Krogstad2,3, Dr. Jared M Allred1
1The University of Alabama, Tuscaloosa, AL, USA. 2Materials Science Division, Argonne National Laboratory, Lemont, IL, USA. 3X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, USA

10:50 - 11:10am
14 Optimizing the dynamic pair distribution function method for inelastic neutron spectrometry of polycrystalline Ni
Kody A. Acosta1, Dr. Helen C. Walker2, Dr. Allyson M. Fry-Petit1
1Department of Chemistry and Biochemistry, California State University-Fullerton, Fullerton, CA, USA. 2ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Oxfordshire, OX11 0QX, United Kingdom

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11:10 - 11:30am
96 Time-resolved total scattering using MeV electrons
Dr. Xijie wang
slac national accelerator laboratory, Menlo Park, CA, USA

3.1.2: Quantum crystallography I

8:30 - 11:30am Monday, 10th July, 2023
Locations Kent A-C
Yu-Sheng Chen, Florian Kleemiss, Krzysztof Wozniak

This Session is dedicated to advances and results obtained in the field of Quantum Crystallography (QCr). QCr involves theoretical and practical aspects of using quantum mechanics during the investigation of crystalline materials. Both directions - the improvement of crystallographic analysis based on quantum mechanical models and the improvement of quantum mechanical methods based on crystallographic data - are covered within this field.

QCr models go beyond the spherical atom approach, ranging from Multipole Models over Hirshfeld Atom Refinement (HAR) to the calculations of experimentally enhanced wavefunctions. They yield better agreement with experimental data and allow for deepened understanding of the properties of materials. Applications for the investigation of intermolecular interactions, bonding indicators, atomic displacement, electronic states, relativistic effects, electron correletion effects, and redistribution of electron density are invited as well as work under non-ambient conditions using these methods. Systems under investigation range from inorganic network structures all the way to large structures such as proteins. This symposium invites crystallographers interested in these new approaches, method developers as well as those who are interested in applications across all experimental techniques (also including X-ray and electron diffaction) and theoretical approaches to obtain high-quality structural, electronic or thermal information.

8:30 - 9:00am
230 The total energy from X-ray electron density?
Professor Lou Massa1, Professor Cherif F. Matta2
1Hunter College & the Graduate School, CUNY, New York, NY, USA. 2Mt. St. Vincent University, Halifax, NS, Canada

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9:00 - 9:30am
237 Aspherical scattering factors from multipole model for X-ray and electron crystallography

Professor Paulina M. Dominiak
University of Warsaw, Warsaw, Masovian Voivodeship, Poland

9:30 - 10:00am
136 Reliability and reproducibility of the determination of physical effects from X-ray constrained wavefunction fitting
PD Dr. Simon Grabowsky
University of Bern, Bern, Bern, Switzerland

10:30 - 11:00am
70 Determination of hydrogen atom position in Stryker's reagent through the application of quantum crystallographic methods on microED data
Dr. Kunal K Jha, Professor Hosea M Nelson
Division of Chemistry & Chemical Engineering, California Institute of Technology, Pasadena, California, USA

11:00 - 11:30am
340 Refinement of anomalous dispersion parameters - more than model improvement
Dr. Michael Bodensteiner
University of Regensburg, Regensburg, Bavaria, Germany

3.1.3: Structural Genomics: Past, Present and Future

8:30 - 11:30am Monday, 10th July, 2023
Locations Laurel CD
Stephen Burley, David Rose

Some 30 years ago, the bold concept of high-throughput determination of macromolecular structures was both visionary and controversial. In retrospect, it set the stage for many of the technical advances that are now standard operating procedures in structural biology, including both biophysical and computational prediction approaches. The goal of this session is to showcase some of the unique contributions of structural genomics in advancing our knowledge of macromolecular structure, accelerating progress in chemical biology and drug discovery, understanding human health and disease, and training structural biology researchers. Talks will include perspectives of past and current Structural Genomics efforts, early-career investigators who got their start through SG, and discussions about how SG will evolve in the coming years.

8:30 - 9:00am
232 Structural Genomics' role in Innovative Structure Characterization
John-Marc Chandonia1, Steven E Brenner1,2
1Environmental Genomics and Systems Biology Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 2Department of Plant and Microbial Biology, University of California, Berkeley, CA, USA

9:00 - 9:30am

76 Structural Genomics from Inside Biopharma and the Future
Executive Director, Bioinformatics & Structural Biology J Michael Sauder
Lilly Biotechnology Center, San Diego, CA, USA

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9:30 - 10:00am
81 20 years of the Structural Genomics Consortium; past achievements and future directions of an open science public-private partnership
Dr. Rachel J Harding
University of Toronto, Toronto, Ontario, Canada. Structural Genomics Consortium, Toronto, Ontario, Canada

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10:30 - 10:45am
212 Challenges of Structural Genomics Two Decades Perspective
Prof. Wladek Minor
University of Virginia, Charlottesville, Va, USA

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10:45 - 11:00am
95 Operations of the National Crystallization Center: Two decades of high-throughput crystallization efforts fueled by structural genomics
Gabrielle R. Budziszewski1, Tiffany R. Wright1, M. Elizabeth Snell1, Miranda L. Lynch1, Sarah E. J. Bowman1,2
1Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA. 2University at Buffalo, Buffalo, NY, USA

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11:00 - 11:30am
215 Structural Genomics: past, present, and future
Dr Andrzej Joachimiak
Structural Biology Center, X-ray Science Division, Argonne National Laboratory,, Argonne, IL, USA. Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL, USA

3.1.4: Small Molecule MicroED I- Expanding Possibilities and Implementation

8:30 - 11:30am Monday, 10th July, 2023
Locations Waterview AB
Daniel Decato, Jessica Bruhn

The emerging field of microcrystal electron diffraction (MicroED), a 3D ED technique, has enabled solving high-resolution crystal structures without the need to grow large crystals and hence has attracted significant interest across various fields. Though MicroED is a relatively new technique, since its initial demonstration it has enabled structure elucidation for a variety of targets that were intractable by other techniques, and it is quickly gaining momentum in the scientific community, with more than 250 unique MicroED structures deposited in the CCDC along with numerous associated publications. This session will focus on examples of how MicroED has been used for structure determination of a variety of samples, highlighting the strengths, future prospects and thereby providing a platform to exchange ideas about

future directions. Talks highlighting industrial applications and the process of establishing core facilities are highly encouraged.

8:30 - 9:00am
93 Crystal structure Determination of Small Molecules by 3D ED/MicroED
Dr. Hongyi Xu
Stockholm University, Stockholm, Stockholm, Sweden. University of Queensland, Brisbane, Queensland, Australia

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9:00 - 9:30am
324 A robust absolute structure determination method by dynamical refinement against electron diffraction data
Lukas Palatinus
Institute of Physics of the CAS, Prague, --, Czech Republic

9:30 - 10:00am
150 MicroED for Metabolomics
Dr. Samantha M. Powell, Dr. Irina V. Novikova, Dr. James E. Evans
Pacific Northwest National Laboratory, Richland, WA, USA

10:30 - 10:50am
278 Electron Diffraction – The Swiss knife among the analytical equipment for solid state characterization for pharmaceuticals
Danny Stam, Dr. Johannes Merkelbach, Dr. Christian Jandl
ELDICO Scientific AG, Villigen, Argau, Switzerland

10:50 - 11:10am
168 XtaLAB Synergy-ED: Single Crystal Structures from Powders
Dr Joseph D Ferrara1, Dr Simon Bates1, Dr Robert Bŭcker2, Michał Jasnowski3, Dr. Mathias Meyer3, Dr. Fraser White4, Dr. Sho Ito5, Dr. Akihito Yamano6, Dr. Yoshitaka Aoyama7, Dr. Eiji Okunishi7
1Rigaku Americas Corp., The Woodlands, TX, USA. 2Rigaku Europe SE, Neu-Isenberf, -, Germany. 3Rigaku Polska, Wrocław, -, Poland. 4Rigaku Europe SE, Neu-Isenberg, -, Germany. 5Rigaku Corporation, Akishima-shi, Tokyo, Japan. 6Rigaku Corporation, Akishima-shi, Tokyp, Japan. 7JEOL Ltd., Akishima-shi, Tokyo, Japan

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11:10 - 11:30am
153 Continuous electron diffraction tomography with Gatan electron counting cameras and Latitude® D
Sahil Gulati, Anahita Pakzad
Gatan, Pleasanton, CA, USA

3.1.5: New Sample preparation technology for cryo-EM and cryo-ET

8:30 - 11:30am Monday, 10th July, 2023

Locations Essex A-C
David Taylor, Jianhua Zhao

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

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498 Voltage gated potassium channels
Shengjie Feng
UCSF, San Francisco, CA, USA

8:30 - 9:00am
59 Efficient tagging of endogenous proteins in human cell lines for structural studies by single particle cryo-EM
Ph.D Wooyoung Choi1, Ph.D Hao Wu1, Ph.D Klaus Yserentant1, Ph.D Bo Huang1,2, Ph.D Yifan Cheng1,3
1UCSF, San Francisco, CA, USA. 23Chan Zuckerberg Biohub, San Francisco, CA, USA. 34Howard Hughes Medical Institute, San Francisco, Ca, USA

9:00 - 9:30am
311 Automated native mass spectrometry screening of membrane proteins for structural biology applications
Natalia de Val1, Scott Kronewitter2, Paul Gazis3, Mick Greer4, Weijing Liu3, Rosa Viner3, Olufemi Adeyemi5, Albert Konijnenberg5, Edward Pryor1
1Thermo Fisher Scientific, Hillsboro, OR, USA. 2Thermo Fisher Scientific, Cambridge, MA, USA. 3Thermo Fisher Scientific, San Jose, CA, USA. 4Thermo Fisher Scientific, Austin, TX, USA. 5Thermo Fisher Scientific, Eindhoven, NL, Netherlands

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10:30 - 11:00am
250 OpenFIBSEM: a universal API for FIBSEM control and automation
Alex de Marco1, Patrick Cleeve2, Lucile Naegele2, Rohit Kannachel2
1NYSBC, New York, NY, USA. 2monash university, clayton, VIC, Australia

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11:00 - 11:30am
362 CryoFIB milling of large tissue samples with on-the-fly localization
Dr Xueming Li
School of Life Science, Tsinghua University, Beijing, Beijing, China

3.1.6: Validating models from the data, other data, and theory

8:30 - 11:30am Monday, 10th July, 2023
Locations Laurel AB
John Rose, Joseph Ferrara

The stakeholders in data management include the scientists and the manufacturers of the instruments producing the data, the caretakers and curators of the data, and the general user community which include members of the preceding groups.

In a perfect world, the raw data and its metadata should be stored in a format that will be readable indefinitely. Should the metadata include the raw data format and version information of the software used to produce the results? Should the processing software (HKL, XDS, DIALS, SHELX* etc.), including any input scripts, be stored in a database for posterity? Should software for downstream analysis, (PHENIX, CCP4, CCP-EM, Olex2, etc.) be stored in the same database, for example? Some disciplines have excellent data management while others do not. For those that do not, what can we do better?
Lastly, how does AI fit into the larger picture data management window?

In this session we will explore the current and future best practices in data management from the perspective of the three stakeholder groups described in the first paragraph. John Helliwell, Chair of the IUCr Committee on Data will give the keynote presentation to open the session

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8:30 - 8:48am
275 Impact on validation and quality of structures deposited to PDB
Wladek Minor, Marcin Cymborowski, David R Cooper
University of Virginia, Charlottesville, VA, USA

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8:48 - 9:06am
125 Data management and data validation best practices from the perspective of a data repository
Dr Matt P Lightfoot, Dr Ian J Bruno, Dr Natalie T Johnson, Yinka Olatunji-Ojo, Suzanna C Ward
Cambridge Crystallographic Data Centre, Cambridge, Cambs, United Kingdom

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9:06 - 9:24am
195 Assuring Quality in Rietveld Refinements
Brian H Toby
Advanced Photon Source, Argonne National Lab, Lemont, IL, USA

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9:24 - 9:42am
252 A comprehensive validation and reassessment of the rutile aristotype's distortion tree using representational analysis and crystal chemistry concepts
Dr. Jared M Allred, Eslam M. Elbakry, Jacob F. Phillips, Top B. Rawot Chhetri
The University of Alabama, Tuscaloosa, AL, USA

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9:42 - 10:00am
280 Raw diffraction data are our ground truth from which all subsequent workflows develop
Emeritus Professor John Richard Helliwell
University of Manchester, Manchester, Manchester, United Kingdom

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10:30 - 10:48am
128 Planning for the future of crystallographic raw data and its metadata

Dr. Herbert J. Bernstein, Frances C Bernstein
Bernstein + Sons, New York, NY, USA

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10:48 - 11:06am
144 Validation and Quality Assessment for Small-Molecule Ligands in the Protein Data Bank
Chenghua Shao1, Jasmine Y Young1, Charmi Bhikadiya2, Ezra Peisach1, Jose M Duarte2, Yana Rose2, Zukang Feng1, wwPDB Team3, Stephen K Burley1
1RCSB Protein Data Bank, Piscataway, NJ, USA. 2RCSB Protein Data Bank, La Jolla, CA, USA. 3Worldwide Protein Data Bank, Piscataway, NJ, USA

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11:06 - 11:24am
333 Validation and archival of MicroED data
Johan Hattne1,2, Michael W Martynowycz2, Max Clabbers2, Johan Unge2, Jieye Lin2, Tamir Gonen1,2,3
1Howard Hughes Medical Institute, University of California, Los Angeles, Los Angeles, CA, USA. 2Department of Biological Chemistry, University of California, Los Angeles, Los Angeles, CA, USA. 3Department of Physiology, University of California, Los Angeles, Los Angeles, CA, USA

PL2 David G. Rognlie Award
11:30am - 12:00pm Monday, 10th July, 2023
Locations Essex A-C

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293 Time-resolved Structural Science
Professor Majed Chergui
Ecole Polytechnique Fédérale de Lausanne, Lausanne, VD, Switzerland

3.2.1: Quantum crystallography II

2:00 - 5:00pm Monday, 10th July, 2023
Locations Kent A-C
Yu-Sheng Chen, Florian Kleemiss, Krzysztof Wozniak

This Session is dedicated to advances and results obtained in the field of Quantum Crystallography (QCr). QCr involves theoretical and practical aspects of using quantum mechanics during the investigation of crystalline materials. Both directions - the improvement of crystallographic analysis based on quantum mechanical models and the improvement of quantum mechanical methods based on crystallographic data - are covered within this field.

QCr models go beyond the spherical atom approach, ranging from Multipole Models over Hirshfeld Atom Refinement (HAR) to the calculation of experimentally enhanced wavefunctions. They yield better agreement with experimental data and allow deepened understanding of the material under investigation. Applications for the investigation of intermolecular interactions, bonding indicators, atomic displacement, electronic states, relativistic effects, electron correlation effects, and redistribution of electron density are invited as well as work under non-ambient conditions using these methods. Systems under investigation range from inorganic network structures all the way to large structures like proteins. This symposium

invites crystallographers interested in these new approaches, method developers as well as these crystallographers who are interested in applications across all experimental techniques (also including X-ray and electron diffraction) and theoretical approaches to obtain high-quality structural, electronic or thermal informant

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2:00 - 2:30pm
213 Extension of Bright Wilson's Justification of the First Hohenberg Kohn Theorem to Non-Nuclear Maxima (NNM)
Chérif F. Matta1, Aldo de Jesus Mortera-Carbonell2, James S. M. Anderson2, Lou Massa3
1Mount Saint Vincent University, Halifax, NS, Canada. 2Universidad Nacional Autonoma de Mexico (UNAM), Mexico, Mexico, Mexico. 3Hunter College, City University of New York (CUNY), NY, NY, USA

2:30 - 3:00pm
40 X-ray Restrained Wavefunction Approach: Latest Achievements and Future Challenges
Dr. Alessandro Genoni
CNRS & University of Lorraine - Laboratory of Theoretical Physics and Chemistry, METZ, GrandEst, France

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3:30 - 4:00pm
85 Charge Density Analyses in Polyimido Sulfur Ligands Yield Single Molecule Magnets
Prof Dietmar Stalke
Georg August Universität Göttingen, Göttingen, Niedersachsen, Germany

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4:00 - 4:30pm
89 Challenges and Capabilities of Quantum Crystallography for Locating Hydrogen Atoms in Transition Metal Hydrides
Dr. Magdalena Woińska, Dr. Sylwia Pawlędzio, Dr. Anna A. Hoser, Dr. Michał L. Chodkiewicz, Prof. Krzysztof Woźniak
Biological and Chemical Research Centre, Chemistry Department, University of Warsaw, Warsaw, Mazovia Voivodship, Poland

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4:30 - 5:00pm
225 Increasing completeness in single-crystal high-pressure diffraction experiments by pre-orienting crystals
Dr Daniel M Tchoń1, Aleksandra Zwolenik2, Dr hab. Anna M Makal2
1Molecular Biophysics and Integrated Bioimaging, Lawrence Berkeley National Laboratory, Berkeley, California, USA. 2Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, Mazovia, Poland

3.2.2: Structure-property relationships of energy materials/Energy density, sustainability

2:00 - 5:00pm Monday, 10th July, 2023
Locations Laurel AB
Alicia Manjon Sanz, Tyger Salters

In pursuit of a sustainable future, structural studies play an important role in the development of functional materials for energy conversion and storage. Crystallography and scattering techniques enable the discovery and elucidation of useful structure-property relationships in crystalline and disordered materials. Such relationships are critical to the design and optimization of batteries, fuel cells, thermoelectric and photovoltaic cells, catalysts, piezoelectric devices, and gas separation technologies, among others. Continuing development of in-situ and in-operando techniques also provide critical understanding of these materials under the conditions of their intended use.

This session will cover emerging interdisciplinary work in the study of materials for energy and sustainability applications, with a focus on how structural studies, both steady-state and time-resolved, lend mechanistic insight into functional material design and optimization.

2:00 - 2:20pm
184 Structure Study of A New Family of Low-Cost Sodium-Ion Battery Cathode
Jue Liu
Oak Ridge National Lab, Oak Ridge, TN, USA

2:20 - 2:40pm
109 The structural study of La0.9Sr0.1Co1-xFexO3-δ through in situ neutron and synchrotron diffraction
Dr. Allyson M Fry-Petit, Dennis Nguyen
California State University, Fullerton, Fullerton, CA, USA

2:40 - 3:00pm
286 Neutron Powder diffraction Studies of Metal-Organic Frameworks for Gas Storage and separation
Dr. Cheng Li
Oak Ridge National Lab, Oak Ridge, TN, USA

3:30 - 4:00pm
211 Octahedral tilting, cation ordering, and hydrogen bonding in layered hybrid halide perovskites
Patrick M Woodward, Noah Holzapfel, Tianyu Liu, Joe Race
The Ohio State University, Columbus, Ohio, USA

4:00 - 4:30pm
84 Structural resolution of H2 and D2 within metal-organic frameworks using neutron diffraction
Hayden Evans1, David Jamarillo2, Brandon Barnett3, Jeff Long2, Craig Brown4, Taner Yildirim4
1NCNR, Gaithersburg, MD, USA. 2University of California Berkeley, Berkeley, CA, USA. 3University of California Berkeley, Berkeley, ca, USA. 4National Institute of Standards and Technology, Gaithersburg, MD, USA

4:30 - 5:00pm
182 Nanostructure transformation as a signature of oxygen redox in Li-rich cathodes
Karena W Chapman

Stony Brook University, Stony Brook, NY, USA

3.2.3: Small Molecule MicroED 2- Expanding Possibilities and Implementation

2:00 - 5:00pm Monday, 10th July, 2023
Locations Waterview AB
Ana Pakzad, Daniel Decato

The emerging field of microcrystal electron diffraction (MicroED), a 3D ED technique, has enabled solving high-resolution crystal structures without the need to grow large crystals and hence has attracted significant interest across various fields. Though MicroED is a relatively new technique, since its initial demonstration it has enabled structure elucidation for a variety of targets that were intractable by other techniques, and it is quickly gaining momentum in the scientific community, with more than 250 unique MicroED structures deposited in the CCDC along with numerous associated publications. This session will focus on examples of how MicroED has been used for structure determination of a variety of samples, highlighting the strengths, future prospects and thereby providing a platform to exchange ideas about future directions. Talks highlighting industrial applications and the process of establishing core facilities are highly encouraged.

2:00 - 2:30pm
172 Expanding the Crystallographer's Toolbox
Justin A. Newman, Luca Iuzzolino, Melissa Tan, Alfred Lee
Merck & Co. Inc., Rahway, NJ, USA

2:30 - 3:00pm
202 Absolute configuration determination of small molecules with MicroED
Bo Wang
Biogen, Cambridge, MA, USA

3:30 - 4:00pm
221 XFEL microcrystal diffraction for fast and accurate small-molecule structures
Daniel W Paley1, Elyse A Schriber2, Aaron S Brewster1, Mariya Aleksich2, Mark Hunter3, Patience A Kotei2, David W Mittan-Moreau1, Vanessa Oklejas1, Raymond G Sierra3, Maggie Ward2
1Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 2University of Connecticut, Storr, CT, USA. 3SLAC National Laboratory, Stanford, CA, USA

4:00 - 4:20pm
104 Structure Determination of Nanocrystalline Metal-Organic Frameworks by MicroED
Dr. Christian Jandl, Dr. Johannes Merkelbach, Dr. Gunther Steinfeld, Danny Stam, Dr. Sebastian Schegk, Dr. Eric Hovestreydt
ELDICO Scientific AG, Villigen, Aargau, Switzerland

4:20 - 4:40pm
185 Mosquito Meets Crystal
Professor Bart Kahr

New York University, NYC, NY, USA

4:40 - 5:00pm
336 XtaLAB Synergy-ED: To cryo, or not to cryo, that is the ED question
Dr. Mark Del Campo1, Dr. Khai-Nghi Truong2, Dr. Robert Bücker2, Dr. Fraser White2, Dr. Tomislav Stolar3, Dr. Krunoslav Užarević3, Dr. Luca Grisanti3, Dr. Ernest Meštrović4, Dr. Mathias Meyer5, Dr. Michał Jasnowski5, Dr. Akihito Yamano6, Dr. Sho Ito6, Dr. Eiji Okunishi7, Dr. Yoshitaka Aoyama7, Dr. Joseph Ferrara1
1Rigaku Americas Corporation, The Woodlands, TX, USA. 2Rigaku Europe SE, Neu-Isenburg, Hesse, Germany. 3Ruđer Bošković Institute, Zagreb, NA, Croatia. 4University of Zagreb, Zagreb, NA, Croatia. 5Rigaku Polska, Wrocław, NA, Poland. 6Rigaku Corporation, Haijima, Tokyo, Japan. 7JEOL Ltd., Akishima, Tokyo, Japan

3.2.4: Complementary BioSAXS and BioSANS Sample Environments

2:00 - 5:00pm Monday, 10th July, 2023
Locations Waterview CD
Hugh O'Neill, Susana Teixeira

Recent and upcoming improvements at synchrotron and neutron sources have fostered interest in the development of new sample environment modalities for biomolecular small-angle scattering (BioSAS) experiments. These are particularly important because of the challenges associated with limited sample availability, polydispersity, enhanced sensitivity of biomolecule solutions to radiation and their environment, which are key aspects in determining the feasibility of BioSAS studies. This session targets both researchers who have never used small angle scattering techniques, interested in learning more about what an experiment entails, and more advanced facility users with an interest in contributing towards developments in sample environment instrumentation. The complementarity of BioSANS and BioSAXS will be discussed in this context, such as automation and machine-learning for industrial formulation discovery, low temperature capabilities for studies of the effects of freezing/thawing, high-pressure induced folding and stability studies, and in-line size-exclusion chromatography for deconvolution of polydisperse samples. We invite a discussion on these and other sample environment developments, as well as new challenges for biomolecular and bio-inspired materials.

2:00 - 2:20pm
270 Biological X-ray Solution Scattering Under Intense Hydrostatic Pressure: Current Applications and Practice
Richard E Gillilan1, Robert C Miller1,2, Gabrielle Ilava1,3, Raley J Schweinfurth1,2, Nozomi Ando2, Qingqiu Huang1
1Center for High Energy X-ray Sciences, Ithaca, NY, USA. 2Cornell University, Ithaca, NY, USA. 3Department of Chemistry, Cornell University, Ithaca, NY, USA

2:20 - 2:40pm
287 Inline Size-Exclusion Chromatography at Bio-SANS
Kevin L. Weiss
Oak Ridge National Laboratory, Oak Ridge, TN, USA

2:40 - 3:00pm
201 Small angle x-ray scattering measurements of protein crowding in the frozen state.
Josue San Emeterio
Xenocs Inc., Holyoke, MA, USA

3:30 - 3:50pm
292 In-situ pressure-temperature studies of biological systems using small-angle neutron scattering technique
Manjula Senanayake, Lilin He, Mark J. Loguillo, Volker S. Urban, Hugh M. O'Neill
Oak Ridge National Laboratory, Oak Ridge, TN, USA

3:50 - 4:10pm
157 Probing Pressure-Driven Protein Phase Behavior via In-Situ High-Pressure Scattering Methods
Brian Paul1,2, Susana CM Teixeira1,2, Eric M Furst1, Abraham M Lenhoff1, Norman J Wagner1
1University of Delaware, Newark, Delaware, USA. 2NIST Center for Neutron Research, Gaithersburg, Maryland, USA

4:10 - 4:30pm
306 Enhanced Sample Environments for Biological SAXS at SSRL BL4-2
Dr Thomas M Weiss
Stanford University, Menlo Park, CA, USA. SSRL, Menlo Park, CA, USA

4:30 - 4:50pm
357 The Autonomous Formulation Laboratory: Automated SAXS and SANS for Formulation Discovery and Optimization
Peter A Beaucage1, Tyler B Martin2
1NIST Center for Neutron Research, Gaithersburg, MD, USA. 2Materials Science and Engineering Division, NIST, Gaithersburg, MD, USA

3.2.5: Hot Structures

2:00 - 5:00pm Monday, 10th July, 2023
Locations Essex A-C
Charles Stewart, Jonathan Clinger

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

2:00 - 2:20pm
87 Structural basis for enzymatic terminal C–H bond functionalization of alkanes

Dr. Qun Liu, Jin Chai, Gongrui Guo, Sean McSweeney, John Shanklin
Brookhaven National Laboratory, Upton, NY, USA

2:20 - 2:40pm
351 Structural characterization of spermidine methyltransferase, a novel member of the plant aminopropyltransferase family from Erythroxylum coca
Dr Charles E Stewart1, Benjamin Chavez2, Dr John C. D'Auria2
1Iowa State University, Ames, IA, USA. 2Leibniz Institute of Plant Genetics and Crop Plant Research, Gatersleben, Saxony-Anhalt, Germany

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2:40 - 3:00pm
68 C-H...O bonds involving Trp sidechain in protein structures
Michal Szczygiel1,2, Harrison Distinguished Professor Wladek Minor1, Professor Zygmunt Derewenda1
1Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, Virginia, USA. 2Department of Computational Biophysics and Bioinformatics, Jagiellonian University, Krakow, Lesser Poland, Poland

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3:30 - 4:00pm
103 Structure of a 10-23 Deoxyribozyme Captured in a Precatalytic State
Evan R Cramer, Sarah A Starcovic, Dr. Aaron R Robart
West Virginia University, Morgantown, WV, USA

4:00 - 4:30pm
83 Crystal structure of LGR ligand α2/β5 from Caenorhabditis elegans with implications for the evolution of glycoprotein hormones
Zhen Gong1, Wei Wang1, Kamel El Omari2, Andrey A Lebedev3, Oliver B Clarke1, Wayne A Hendrickson1
1Columbia University, New York, NY, USA. 2Diamond Light Source, Didcot, Oxfordshire, United Kingdom. 3CCP4, Didcot, Oxfordshire, United Kingdom

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4:30 - 5:00pm
111 Visualizing protonation states in serine hydroxymethyltransferase with neutron crystallography
Victoria N Drago1, Claudia Campos2, Mattea Hooper2, Aliyah Collins2, Oksana Gerlits2, Kevin L Weiss1, Matthew P Blakeley3, Robert S Phillips4,5, Andrey Kovalevsky1
1Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2Department of Natural Sciences, University of Tennessee Wesleyan, Athens, TN, USA. 3Large Scale Structures Group, Institut Laue-Langevin, Grenoble, N/A, France. 4Department of Chemistry, University of Georgia, Athens, GA, USA. 5Department of Biochemistry and Molecular Biology, University of Georgia, Athens, -, USA

3.2.6: Structure of nucleic acid

2:00 - 5:00pm Monday, 10th July, 2023

Locations Laurel CD
Yuan He, Melanie Ohi

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

2:00 - 2:30pm
295 Histone H2B ubiquitination in transcription regulation
Dr. Cynthia Wolberger
Johns Hopkins University School of Medicine, Baltimore, MD, USA

2:30 - 3:00pm
206 Nanoarchitectural engineering of RNA for structural determination using cryo-EM
Prof. Peng Yin, Di Liu
Harvard University, Boston, MA, USA

3:30 - 4:00pm
378 Lesion recognition by XPC, TFIIH and XPA in DNA Excision Repair
Dr. Wei Yang1, Dr. Jin Seok Kim1, Dr. Xuemin Chen2, Dr. Yanxiang Cui1, Dr. Filip M. Golebiowski11, Dr. Huaibin Wang1, Dr. Fumio Hanaoka3, Dr. Kaoru Sugasawa4
1NIH, Bethesda, MD, USA. 2Anhui University, Hefei, Anhui, China. 3NIG, Mishima, Shizuoka, Japan. 4Kobe University, Kobe, Hyogo, Japan

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4:00 - 4:20pm
298 Group II Intron Splicing Mechanisms - Ribozymes and Retrotransposons
Dr. Ling Xu1,2, Kevin Chung1, Tianshuo Liu1, Pengxin Chai1, Dr. Junhui Peng3, Dr. Swapnil Devarkar1, Dr. Anna Pyle1,2
1Yale University, New Haven, CT, USA. 2HHMI, Chevy Chase, MD, USA. 3Rockefeller University, New York, NY, USA

4:20 - 4:40pm
231 CryoEM reveals the mechanism of mediator driven Rad51 filament formation in Homologous recombination.
Dr Jaigeeth Deveryshetty1, Dr Rahul Chadda1, Ms Jenna Mattice2, Mr Micheal Rau3, Ms Simrithaa Karunakaran1, Dr Nilisha Pokhrel4,5, Mr Noah Englander1, Prof James Fitzpatrick3,6, Prof Brian Bothner2, Prof Edwin Antony1
1Saint Louis University, St.Louis, MO, USA. 2Montana state University, Bozeman, Montana, USA. 3Washington University at St.Louis, St.Louis, MO, USA. 4Marquette University, Milwaukee, WI, USA. 5Laronde Bio, Boston, MA, USA. 6Roche, Basel, Schweiz, Switzerland

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4:40 - 5:00pm

129 Cryo-EM Structures of the DEAH-box Helicase DHX36 Reveals the Initiation of Unwinding DNA and RNA G-quadruplexes
Michael T Banco1, Tapas Paul2, Jiansen Jiang1, Sua Myong2, Adrian R Ferré-D'Amaré1
1National Heart, Lung and Blood Institute, Bethesda, MD, USA. 2Johns Hopkins University, Baltimore, MD, USA

Poster Session #3

5:30 - 7:30pm Monday, 10th July, 2023
Locations Exhibit Hall

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436 NERSC-In-The-Loop: Supporting Experimental Facilities At The National Energy Research Scientific Computing Center.
Dr Bjoern Enders
Lawrence Berkeley Natonal Lab, Berkeley, CA, USA

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432 EMhub: a web platform for CryoEM centers management and on-the-fly data processing
Dr José Miguel De la Rosa Trevín1, Dr Grigory Sharov2, Dr Israel Fernández1, Dr Marta Carroni3
1St. Jude Children's Research Hospital, Memphis, Tennessee, USA. 2Laboratory of Molecular Biology, Cambridge, Cambridge, United Kingdom. 3Science for Life Laboratory, Stockholm, Stockholm, Sweden

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412 Sample preparation for routine and advanced structural biology, including serial data collection, microED, and cryoEM
Mr Stefan Kolek1, Mr Patrick Shaw Stewart1, Mr Jack Stubbs2, Mr Peter Baldock1
1Douglas Instruments Ltd, Hungerford, Berkshire, United Kingdom. 2Southampton University, Southampton, Hampshire, United Kingdom

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411 Investigating the role of a highly conserved tryptophan in the copper-binding site of Bacillus subtilis YcnI protein
Yuri R. O. Silva, Dia Zheng, Oriana S. Fisher, Stephen C Peters
Lehigh University, Bethlehem, PA, USA

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410 3D structures of reduced state NADH-ferredoxin reductase (BphA4) solved in X-ray crystallography and cryo-EM
Akira Shinoda Takasu, Miki Senda, Aramaki Shinji, Toshio Moriya, Toshiya Senda
KEK, Tsukuba, Ibaraki, Japan

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404 Crystals of new bis-2ampy Ni(II) compounds with TCNQ or TCNQF4. Unexpected structural differences.
Dr. Milagros Tomás1,2, Prof. Irene Ara1,2, Prof. Juraj Černák3, Prof. Larry R. Falvello4,2, María Rubio1, Dr. Slavomíra Šterbinská4,2
1Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), Departamento de Química Inorgánica, Zaragoza, Zaragoza, Spain. 2CSIC-Universidad de Zaragoza, Zaragoza, Zaragoza, Spain. 3P. J. Šafárik University in Košice, Faculty of Sciences, Institute of Chemistry, Department of

Inorganic Chemistry, Košice, Slovakia, Slovakia. 4Instituto de Nanociencia y Materiales de Aragón (INMA) and Departamento de Química Inorgánica, Zaragoza, Zaragoza, Spain

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403 Reaction of Monosaccharides with Substituted Anilines and Phenylhydrazines: Schiff Bases vs. Glycosylamines as Crystalline Products
William H. Ojala, Andrew B. Smith, Alexandra C. Korte, Leah R. Streitman, Jenna A. Vargason, Jonathan M. Smieja
University of St. Thomas, St. Paul, Minnesota, USA

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402 The Berkeley Center for Structural Biology at the Advanced Light Source
Marc Allaire1, Jeff Dickert1, John Taylor1, Randall Cayford1, Kevin Royal1, Anthony Rozales1, Daniel Santos1, Staey Ortega1, Adrian Spucces1, Troy Stevens1, Antoine Wojdyla1, Jay Nix2, Yang Ha1, Daniil Prigozhin1
1Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 2Molecular Biology Consortium, Berkeley, CA, USA

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397 The structural basis for macaque Fc α receptor (CD89) activation by IgA Fc
William D. Tolbert, Pratibha Gurung, Rebekah Sherburn, Suneetha Gottumukkala, Marzena Pazgier
Department of Medicine of Uniformed Services University of the Health Sciences, Bethesda, Maryland, USA

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381 A case of UV-induced proton-coupled electron transfer in Copper-doped Zinc Creatinine Sulfate: An EPR, DFT, and Crystallographic Investigation
Dr Michael J Colaneri1, Dr Simon J Teat2, Dr Jacqueline Vitali3
1SUNY at Old Westbury, Old Westbury, NY, USA. 2Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 3Cleveland State University, Cleveland, OH, USA

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379 Dihydroorotase from Methanococcus jannaschii with substrate and product bound
Dr. Jacqueline Vitali1, Dr. Jay C Nix2, Ms. Haley E Newman1, Dr. Michael J Colaneri3
1Cleveland State University, Cleveland, OH, USA. 2Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 3SUNY at Old Westbury, Old Westbury, NY, USA

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369 Learning how science works with crystals: A proposal for Africa
Dr. Joy W Kiano1, Dr. Patricia W Gitari2, Ms Lillian Nyaranga3, Prof. Juan M. Garcia-Ruiz4
1Nemayiana, Africa Museum of Science and Technology), Nairobi, Kenya, Kenya. 2A.E.S.A, Nairobi, Kenya, Kenya. 3Elimu Shop, Nairobi, Kenya, Kenya. 4Instituto ANdaluz de Ciencias de la Tierra. CSIC-Universidad de Granada, Granada, Andalucia, Spain

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364 Dissemination of cryoEM best practices by training with modular units called “Merit Badges”
Christina M Zimanyi, Edward T. Eng, Jeffrey S Kieft, Alex de Marco
National Center for CryoEM Access and Training, Simons Electron Microscopy Center, New York Structural Biology Center, New York, NY, USA

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354 Structural insights for β-lactam antibiotics
Prof. Lin-Woo Kang

Konkuk University, Seoul, MD, Korea, Republic of

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353 Unravelling the dynamics of biomolecules by serial crystallography at X-ray Free Electron Lasers
Petra Fromme
Arizona State University, Tempe, AZ, USA

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341 A Complete, Versatile, and Cost-Effective Solution for Routine Serial and "Conventional" Synchrotron Crystallography
Robert E Thorne
MiTeGen, LLC, Ithaca, NY, USA

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320 Equilibrium and time-resolved SAXS at BioCAT
Maxwell B Watkins, Jesse Hopkins, Richard Heurich, Weikang Ma, Carrie Clark, Mark Vukonich, Thomas Irving
BioCAT/IIT, Argonne, IL, USA

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217 Public use CryoEM at SPring-8
Ph.D. Hideki \ Shigematsu1,2, Ph.D. Christoph Gerle2, Ph.D. Chai Gopalasingam2
1Japan Synchrotron Radiation Research Institute, Sayo-gun, Hyogo, Japan. 2RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan

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207 SER-CAT Data Collection Plans at Other Beamlines During APS Dark Period
Zhongmin Jin1,2, John Chrzas1,2, John P Rose1,2, Unmesh Chinte1,2, Palani Kandavelu1,2, Roderick C Salazar1,2, Zheng-Qing Fu1,2, B.C. Wang1,2
1SER-CAT, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, USA. 2Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA, USA

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180 Approximate Symmetry in P2 and C2 Organic Structures
Professor Carolyn P Brock
University of Kentucky, Lexington, KY, USA

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97 Allosteric activation of choanoflagellate soluble guanylate cyclases
William C Thomas, Yang Wu, Michael A Marletta
University of California, Berkeley, Berkeley, CA, USA

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53 Structural and Functional Studies on a F-like Type IV Secretion System Protein TrbB
Arnold Apostol, Gerald F Audette
Centre for Research on Biomolecular Interactions, Department of Chemistry, York University, Toronto, ON, Canada

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44 Exploring the limits of 2D template matching for detecting targets in cellular cryo-EM images
Kexin Zhang
The University of Massachusetts Chan Medical School, Worcester, Massachusetts, USA

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291 Integrated M and RELION pipeline in a Linux environment
Zhihai Liu, Jinhong Wang, Hua Wang, Lin Mei
Single Particle LLC, Mission Viejo, CA, USA

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339 The GM/CA@APS Structural Biology Facility Upgrade Plan and APS-Upgrade
Dr. Robert F Fischetti1, Dr. Nagarajan Venugopalan1, Dr. Michael Becker1, Stephen Corcoran1, Dale Ferguson1, Mark Hilgart1, Dr. David J Kissick1, Dr. Oleg Makarov1, Dr. Craig M Ogata1, Dr. Sergey Stepanov1, Dr. Qingping Xu1, Dr. Shenglan Xu1, Professor Janet L Smith2
1Argonne National Laboratory/APS, Lemont, IL, USA. 2Life Sciences Institue, University of Michigan, Ann Arbor, MI, USA

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430 The Structural Molecular Biology Program at the Stanford Synchrotron Radiation Lightsource
Silvia Russi, Derek A Mendez
SLAC National Accelerator Laboratory, Menlo Park, CA, USA

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443 Advancing Crystallography Research: The Latest Progress and Future Directions of NE-CAT Beamlines at the Advanced Photon Source
Ali Kaya, Malcolm Capel, Igor Kourinov, Anthony Lynch, Frank Murphy, David Neau, Kay Perry, Jonathan Schuermann, Narayanasami Sukumar, James Withrow, Steve Ealick
Department of Chemistry and Chemical Biology, Cornell University / NE-CAT, Lemont, IL, USA

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319 What to do when h, k and l do not describe all the reflections in the diffraction pattern?
Dr. Jessica Bruhn
NanoImaging Services Inc., San Diego, CA, USA

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330 Further studies on copper-cyanide networks
Dr. Peter WR Corfield, Alvin M F Varona, Tristan B DaCunha, Nurul B Eisha, Ahmed Elsayed
Chemistry Dept., Fordham University, The Bronx, NY, USA

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344 Copper Acetate Small Molecule Crystallography Undergraduate Experiments
Mr. Alain M Beauparlant, Dr. Sandy Eagle, Mr. Malachi o Cope, Ms. Alandria R Marshall
East Tennessee State University, Johnson City, TN, USA

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204 Structural Changes on Silicon-Graphite Anodes for Lithium-Ion Batteries by In-Situ Synchrotron X-ray Diffraction
Eng Weicheng Hua1, Msc Pedro A Sanchez2, Dr Javier Campo Ruiz3, Dr Federico H Cova4, Dr Maria V Blanco2
1Norwegian University of Science and Technology, Trondheim, Tronderlag, Norway. 2University of Zaragoza, Zaragoza, Aragon, Spain. 3CSIC, Zaragoza, aragon, Spain. 4ALBA Synchrotron, Barcelona, Barcelona, Spain

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8 Analysis of Hasse Diagrams of Crystallographic Point Groups Determines Surprising Crystal System Relationships
Maureen M. Julian1, Matthew Macauley2
1Virginia Tech, Blacksburg, VA, USA. 2Clemson University, Clemson, SC, USA

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91 In situ structures of secretins from bacterial type II secretion system reveal their membrane interactions and translocation process
Dr. Zhili Yu1, Dr. muyuan chen1,2, Dr. Tong Huo1, Dr. Steven J. Ludtke1,3, Dr. zhao wang1,3
1baylor college of medicine, houston, TX, USA. 2SLAC National Accelerator Laboratory, Menlo Park, California, USA. 3cryoEM/ET core at BCM, houston, TX, USA

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473 CryoEM SPA for Structural Understanding of A-to-I RNA Editing: Human Adenosine Deaminase Acting on RNA 2 (ADAR2) Complexed with dsRNA
Mellissa Matthrew1, Alexander Thuy-Boun2, Sukanya Mozumder2, Peter A Beal2, Andrew J Fisher2
1Okinawa Institute of Science and Technology, Davis, CA, USA. 2UC Davis, Davis, CA, USA

3.3.1: Would You Publish This?

7:30 - 9:00pm Monday, 10th July, 2023
Locations Kent A-C
Rebecca McAuliffe, Matthew Brown

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

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500 A crystal of tetrakis(acetato) dirhodium(II)
Alain Beauparlant
East Tennessee State University, Johnson City, TN, USA

7:30 - 7:40pm
135 Strategies to find low-occupancy ligands in a protein-peptide crystal
Dana J Sowa1,2, Sara N Andres1,2
1McMaster University, Hamilton, ON, Canada. 2Michael DeGroote Institute for Infectious Disease Research, Hamilton, ON, Canada

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7:40 - 7:50pm
192 You Would Think 1.2 Angstrom Resolution Would be Enough for Structure Solution …
Gerald F Audette

York University, Toronto, ON, Canada

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7:50 - 8:00pm
256 How Should You Publish This? Thoughts from an Acta C Editor.
Dr. Amy A. Sarjeant1, Prof. Larry Falvello2, Prof. Alan R. Kenedy3, Prof. Paul R. Raithby4, Prof. Jonathan M. White5
1Bristol Myers Squibb, New Brunswick, NJ, USA. 2Universidad de Zaragoza, Plaza San Francisco, Zaragoza, Spain. 3University of Strathclyde, Glasgow, Scotland, United Kingdom. 4University of Bath, Bath, England, United Kingdom. 5The University of Melbourne, Melbourne, Victoria, Australia

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8:00 - 8:10pm
269 Can't we just use Squeeze?
Nichole R Valdez
Sandia National Laboratories, Albuquerque, NM, USA

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8:10 - 8:20pm
314 Optimizing data collection time for absolute configuration determination
Ashley Weiland
Bruker AXS LLC, Madison, WI, USA

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8:30 - 8:40pm
138 "I can't do that, Dave": Machine-Learning language in Scientific Publications.
David R Rose
University of Waterloo, Waterloo, Ontario, Canada

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8:40 - 8:50pm
344 Copper Acetate Small Molecule Crystallography Undergraduate Experiments
Mr. Alain M Beauparlant, Dr. Sandy Eagle, Mr. Malachi o Cope, Ms. Alandria R Marshall
East Tennessee State University, Johnson City, TN, USA

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8:50 - 9:00pm
98 When Is PXRD Data Good Enough, Or When Should I Stop Trying To Resolve Those Tiny Peaks Out Of The Baseline?
Dr. Matthew L. Brown
University of British Columbia, Kelowna, BC, Canada

PL4 Wood Award
7:30 - 9:30pm Monday, 10th July, 2023
Locations Essex A-C

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243 Exploring the impact of crystals on mind and art
Professor Juan M Garcia-Ruiz
Instituto Andaluz de Ciencias de la Tierra. CSIC-Universidad de Granada, Granada, Andalucía, Spain

Tuesday, July 11, 2023

4.1.1: The Economics of Structural Science, in Memory of Carlos Murillo

8:30 - 11:30am Tuesday, 11th July, 2023
Locations Kent A-C
Larry Falvello, Brian Mahon, Dubravka Sisak Jung
Scientists cannot escape the restraint imposed by the cost of their research. This session examines the past, current, and future states of funding and profit in the world of structural sciences, which covers structural biology and materials science. Researchers currently need to navigate an ecosystem of resources which span academia, industry, government, and non-profit agencies. Topics include: How does funding drive the need and availability of structural scientific results? Why support structural science? Funding a service lab and justifying the cost. How does a contract research lab make services economically feasible? Also, how do young investigators leverage the movement of government agencies funding centralized national centers or regional cores?

This session is offered in memory of Carlos A. Murillo (died Nov. 6, 2021) who spoke in this session when it was called Economics of Crystallography in 2021. Carlos led the NSF Chemistry Instrumentation program. There he supported developing new techniques and capabilities for research and promoting diversity in the structural sciences. He oversaw ChemMatCARS, a national synchrotron X-ray facility, was a founding member of the National Academy of Sciences of Costa Rica, and a fellow of AAAS. Carlos was a strong advocate for crystallography and its ability to the advance our scientific knowledge.

8:40 - 9:00am
240 The cost of big science
Prof Javier CAMPO
Aragon Nanoscience and Materials Institute (CSIC-University of Zaragoza), Zaragoza, 50009, Spain

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9:00 - 9:20am
220 Economics of Biodata Archiving Viewed Through the Lens of the RCSB Protein Data Bank
Professor Stephen K Burley
RCSB Protein Data Bank, Piscataway, NJ, USA

9:20 - 9:40am
267 Considerations for running a dedicated Cryo-EM Core facility
William J Rice
NYU Langone, New York, NY, USA

9:40 - 10:00am
281 MetalJet - Making the Impossible Possible
Dr. Julius Hållstedt
Excillum, Kista, -, Sweden

10:30 - 10:50am
265 The Role of the NSF's ChemMatCARS Advanced Crystallography Program in the Economic Crystallography
Professor Yu-Sheng Chen1, Dr. Tieyan Chang Chang1, Dr. Ying-Ping Chen2,1
1University of Chicago, Chicago, IL, USA. 2University of CHicago, Chicago, IL, USA

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10:50 - 11:10am
276 Innovating Together: How Strategic Academic-Industry Collaboration can Drive Advances in Materials Discovery and Create Economic and Socio-economic Benefits
Prof. Nick Vukotic, Dr. Anton Dmitrienko
University of Windsor, Windsor, Ontario, Canada

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11:10 - 11:30am
64 Assessing the Value of Small Molecule Service Crystallography in the Face of Advancing Technology
Steven P. Kelley
University of Missouri-Columbia, Columbia, MO, USA

4.1.2: SAS in Vaccines and Drug Delivery Systems

8:30 - 11:30am Tuesday, 11th July, 2023
Locations Waterview AB
Suzette Pabit, Alice Thwin

Small-Angle X-ray scattering and Neuron Scattering are well-established experimental techniques that allow for structural characterization of biomaterials in solution under physiologically relevant conditions. These techniques allow for the acquisition of relevant data in real world conditions and has the potential to accelerate the development of biopharmaceutical products. SAXS and SANS can give nanometer and sub-nanometer structure information to help optimize pharmaceutical efficacy on a timescale not seen before. This session will highlight both success stories where SAS techniques were used for the development of vaccines, antibodies and drug delivery systems and at the same time address current considerations and challenges in using SAS for drug product development.

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8:30 - 8:50am
190 Investigating temperature and pH-dependent phase behavior of lipid nanoparticles with small angle X-ray scattering.
Josue San Emeterio
Xenocs Inc., Holyoke, Ma, USA

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8:50 - 9:10am
302 Exploring the structure of lipid nanoparticle-based mRNA vaccine systems using a laboratory SAXS beamline
Dr. Heiner Santner, Dr. Heike Ehmann
Anton Paar, Graz, Styria, Austria

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9:10 - 9:35am
147 Redefining the characterization paradigm of RNA lipid nanoparticles
Sarah J Shepherd, Dr. Marshall S Padilla, Dr. Kushol Gupta, Dr. David Issadore, Dr. Michael J Mitchell
University of Pennsylvania, Philadelphia, PA, USA

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9:35 - 10:00am
42 High-Throughput Small Angle X-ray Scattering (HT-SAXS) Pipeline for Lipid Nanoparticle (LNP) Development at the SIBYLS Beamline
Dr. Lee Joon Kim1, Dr. Michal Hammel1, Dr. Greg L. Hura1,2
1Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 2University of California Santa Cruz, Santa Cruz, CA, USA

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10:30 - 11:00am
181 Preservative-induced micelle formation of poloxamer 188
Dr. Rachel R Ford
NIST Center for Neutron Research, Gaithersburg, MD, USA

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11:00 - 11:30am
307 Structural characterization of two-compartment lipid nanoparticles using small-angle x-ray/neutron scattering
Dr. Wellington C Leite1, Dr. Jacob L Thelen2, Dr. Volker Urban1, Dr. Hugh O'Neill1, Dr. Alexander Grishaev3, Dr. Joseph E Cutis4, Dr. Susan T. Krueger4, Dr. Maria M. Castellanos5
1Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2Exponent Inc, Seattle, WA, USA. 3Institute for Bioscience and Biotechnology Research, Maryland, MD, USA. 4NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, USA. 5GSK, Rockville Center for Vaccines Research, Rockville, MD, USA

4.1.3: Structure Based Drug Design

8:30 - 11:30am Tuesday, 11th July, 2023
Locations Essex A-C

Elizabeth Sprague, Alice Thwin, Sandra Gabelli
In this session we will feature applications of structural biology methods to drug discovery. Possible topics may include structure/function studies to inform drug discovery, hit validation, lead optimization challenges and fragments with a particular interest in examples involving a variety of techniques (e.g. xray, NMR, EM, in silico, biophysics, etc). Technology or methods development in these areas is also of interest.

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8:30 - 8:55am
360 Molecular glue induced targeted protein degradation
Matthew Clifton
Novartis, Emeryville, CA, USA

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8:55 - 9:20am

161 Drug discovery targeting GTP metabolism for cancer and infectious diseases using X-ray crystallography and cryo-EM
Prof. Toshiya Senda1,2,3, Prof. Koh Takeuchi4, Prof. Atsuo T Sasaki5,6,7
1High Energy Accelerator Research Organization, Tsukuba, Ibaraki, Japan. 2Sokendai, Tsukuba, Ibaraki, Japan. 3U. Tsukuba, Tsukuba, Ibaraki, Japan. 4U. Tokyo, Hongo, Tokyo, Japan. 5U. Cincinnati, Cincinnati, OH, USA. 6Keio U., Tsuruoka, Yamagata, Japan. 7Hiroshima U., Hiroshima, Hiroshima, Japan

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9:20 - 9:45am
112 Fragment-based screening approach reveals non-orthosteric pockets in the search for allosteric inhibitors of tau-tubulin kinase 1
Robert P Hayes1, Edward DiNunzio2, Mahdieh Yazdani3, Justyna Sikorska2, Yili Chen2, Sriram Tyagarajan2, Younghee Park2, Amy Lee3, Cesar Reyes3, Daniel Burschowsky4, Matthias Zebisch4, Yangsi Ou3, Marina Bukhtiyarova3, Shahriar Niroomand3, Yuan Tian3, Shawn Stachel3, Hua Su3, Jacqueline D Hicks2, Daniel F Wyss2
1Merck, Boston, MA, USA. 2Merck, Kenilworth, NJ, USA. 3Merck, West Point, PA, USA. 4Evotec, Abingdon, Oxfordshire, United Kingdom

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9:45 - 10:00am
110 Hiding in plain sight: distilling protein-ligand hotspots from hundreds of Hsp90 crystal structures
Timothy R Stachowski, Marcus Fischer
St. Jude Children's Research Hospital, Memphis, TN, USA

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10:30 - 10:50am
9 In situ refinement restraints from quantum mechanical methods
Dr Nigel W Moriarty1, Dr Dorothee C Liebschner1, Dr Billy K Poon1, Dr Paul D Adams1,2
1Lawrence Berkeley Lab, Berkeley, CA, USA. 2University of Califonrnia, Berkeley, Berkeley, CA, USA

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10:50 - 11:10am
282 Uncovering the molecular basis for SARM1 activation
Dr Philip S Kerry1, Dr Andrew Brearley1, Dr Marieke Furrer2, Dr Katie Cunnea1
1Evotec, Abingdon, Oxfordshire, United Kingdom. 2Evotec, Hamburg, Germany, Germany

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11:10 - 11:30am
141 Cryo-EM Structure of a Voltage-gated Potassium Channel Kv3.1 in Complex with a Novel Potentiator Reveals a New Binding Site Suggesting the Mechanism of Action
Yun-Ting Chen, Mee Ra Heo, Xin-Jun Zhang, James Kostas, Yuxing Li, Richard Kraus, Vincent Santarelli, Yacob Gomez-Llorente, Daniel Klein, Anthony Ginnetti, Michael Marino, Shawn Stachel, Andrii Ishchenko
Merck and Co., Inc., West Point, PA, USA

4.1.4: One Weird Trick

8:30 - 11:30am Tuesday, 11th July, 2023

Locations Laurel CD
Jonathan Hermann, Charles Bou-Nader

Structural scientists approach experimentation through a uniquely empirical lens, one often dominated by trial and error. As such, the success or failure of a structural technique can sometimes rely on small experimental details which may initially appear unintuitive or unimportant. Rather than relegate these important details to a strategic sentence or two within a manuscript's methods section, this session aims to highlight these unexpected methodological advances in structural science workflows. As structural techniques evolve faster than ever to adapt to new technologies and samples, this session will feature practical developments that may or may not warrant a formalized manuscript, but nevertheless were essential to the success of a structural investigation

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9:00 - 9:30am
162 The structure of the translating bacterial ribosome at 1.55 Å resolution
Dr Simon Fromm1, Kate Marie O'Connor2, Dr Michael Purdy3, Dr Pramod R. Bhatt2, Dr Gary Longharn2, Dr John F Atkins2, Dr Ahmad Jomaa3, Dr Simone Mattei1
1EMBL Heidelberg, Heidelberg, NA, Germany. 2University College Cork, Cork, NA, Ireland. 3University of Virginia, Charlottesville, VA, USA

9:30 - 10:00am
186 Crystal structures of replication-linked RNAs from enteroviral genomes
Assistant Professor Deepak Koirala
University of Maryland Baltimore County (UMBC), Baltimore, Maryland, USA

10:30 - 11:00am
122 Virtual Reality as a thinking tool for structural investigation
Dr. Martina Maritan
Nanome, San Diego, CA, USA

11:00 - 11:30am
223 Native structure of mosquito salivary protein uncovers domains relevant to pathogen transmission
Shiheng Liu
UCLA, Los Angeles, California, USA

4.1.5: Exploring Intermolecular Forces and Interactions

8:30 - 11:30am Tuesday, 11th July, 2023
Locations Laurel AB
Perter Corfield, Joe Reibenspies
This session will explore how crystal structures can be used to understand intermolecular forces and interactions. Talks focusing either on tools (such as CrystalExplorer) or specific case studies are welcome

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8:30 - 9:00am

18 How can we use intermolecular interactions in crystals? Lattice energies, predicting crystal growth and more…
Dr. Peter R Spackman1, Prof. Mark A Spackman2, Prof. Julian D Gale3
1Curtin Institute for Computation, School of Molecular and Life Sciences, Curtin University, Perth, WA, Australia. 2School of Molecular Sciences, University of Western Australia, Perth, WA, Australia. 3Curtin Institute for Computation, School of Molecular and Life Sciences, Perth, WA, Australia

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9:00 - 9:30am
154 Non-covalent Interactions and Morphologies As Tools for Structure Driven Informatics: Rationalizing the Behavior of Ionic Liquids
Dr Patrick C Hillesheim1, Dr Arsalan Mirjafari2, Dr Matthias Zeller3, Sophia Bellia1, Mairead Boucher1
1Ave Maria University, Ave Maria, Florida, USA. 2SUNY Oswego, Oswego, NY, USA. 3Purdue University, West Lafayette, Indiana, USA

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9:30 - 10:00am
115 Utilizing Data-Driven Tools to Investigate the Relative Stability of Solid Forms
Dr. Jeff W Lengyel1, Dr. Ghazala Sadiq2
1Cambridge Crystallographic Data Centre, Boston, MA, USA. 2Cambridge Crystallographic Data Centre, Cambridge, N/A, United Kingdom

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10:30 - 10:45am
253 Syntheses, crystal structures and Hirshfeld surface analysis of three salts of 1-(4-nitrophenyl)piperazine
Sreeramapura D. Archana,1, Sabine Foro2, Hemmige S. Yathirajan,1, Haruvegowda Kiran Kumar,1, Ray J. Butcher3, Rishik Balerao4
1University of Mysore, Mysore-570 006, Karnataka, India. 2Darmstadt University of Technology, Darmstadt, Hesse, Germany. 3Howard University, Washington, DC, USA. 4cThomas Jefferson High School for Science and Technology, Alexandria, VA, USA

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10:45 - 11:00am
99 Novel Nickel(II) Complex with a Thiosemicarbazide: Synthesis, Structure and Noncovalent Interactions
Gustavo Jones Lima, Professor Claudia Cristina Gatto
University of Brasilia, Brasília, DF, Brazil

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11:00 - 11:15am
57 Understanding Physical and Chemical Interactions Deriving Polymer-Metal-Organic Framework Gel Formation for Drug Delivery
Prince Verma, Mark Bannon, Mara Kuenen, Rachel Letteri, Gaurav Giri
University of Virginia, Charlottesville, VA, USA

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11:15 - 11:30am
271 Hydrogen-Bonded Frameworks for Molecular Structure Determination

Dr. Tony HU
New York University, NYC, NY, USA

4.1.6: Magnetism, symmetry, and electronic correlations in topological materials and other quantum systems.

8:30 - 11:30am Tuesday, 11th July, 2023
Locations Waterview CD
Keith Taddei, Jared Allred

This session will focus on the central importance of symmetries in determining the properties of topological and quantum materials. Talks will focus on time reversal symmetry breaking, symmetry protection and the corresponding exotic correlated electron and topological states they can enforce such as magnetic insulators, Weyl/Dirac semimetals, topological superconductivity, quantum spin liquids, and quantum magnetism.

8:30 - 9:10am
285 The geometrically frustrated spin glass (Fe1-pGap)2TiO5
Dr Daniel Phelan1, Dr Feng Ye2, Hong Zheng1, Elena Krivyakina1,3, Anjana Samarakoon1, Patrick LaBarre4, Jennife Neu5,6, Theo Siegrist7,8, Stephan Rosenkranz1, Sergey Syzranov4, Authur Ramirez4
1ANL, Lemont, IL, USA. 2ORNL, Oak Ridge, TN, USA. 3Northern Illinois University, DeKalb, IL, USA. 4UCSC, Santa Cruz, CA, USA. 5FSU, Tallahassee, FL, USA. 6Nuclear Nonproliferation Division, Oak Ridge, TN, USA. 7NHMFL, Tallahassee, FL, USA. 8FAMU-FSU College of Engineering, Tallahassee, FL, USA

9:10 - 9:35am
289 Understanding the local spin structure of MnPSe3 and MnPS3 through magnetic pair distribution function analysis
Raju Baral1, Jue Liu1, Nan Huang2, David Mandrus2, Stuart Calder1
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2University of Tennessee, Knoxville, TN, USA

9:35 - 10:00am
71 A magnetic excitation linking quasi-1D Chevrel-type selenide and arsenide superconductors
Tyra Douglas1, Songxue Chi2, Keith Taddei2, Jared Allred1
1University of Alabama, Tuscaloosa, AL, USA. 2Oakridge National Laboratory, Oakridge, TN, USA

10:30 - 10:55am
323 Coupling of charge density wave to a spin cycloid in topological semimetal NdSbxTe2−x−δ
Tyger H Salters1, Dr Fabio Orlandi2, Dr. Tanya Berry1, Dr. Jason F Khoury1, Dr. Pascal Manuel2, Dr. Leslie M Schoop1
1Princeton University, Department of Chemistry, Princeton, New Jersey, USA. 2ISIS Neutron Pulsed Facility, Rutherford Appleton Laboratory, Oxford, Oxfordshire, United Kingdom

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10:55 - 11:20am
169 Zig-Zag ground state and Kitaev interactions in the spin-1 honeycomb material KNiAsO4
Keith M Taddei1, Ovi Garlea1, Anjana Samarakoon2, Duminda Sanjeewa3, Jie Xing4, Thomas Heitmann3, Clarina dela Cruz1, Athena Sefat1, David Parker1
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2Argonne National Laboratory, Lemont, IL, USA. 3MIRR, Columbia, MO, USA. 4University of South Carolina, Columbia, SC, USA

PL3 Patterson Award

11:30am - 12:30pm Tuesday, 11th July, 2023
Locations Essex A-C

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472 Structure of Membrane Protein's
Tamir Gonen
HHMI/UCLA, Los Angeles, CA, USA

4.2.1: Small Molecule Crystal Structures in Drug Product Design

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Essex A-C
Amy Sarjeant, Rajni Bhardwaj

Crystal engineering is one of the key approaches which is utilized in pharmaceutical industries to obtain optimum drug product. The arrangement of molecules of active pharmaceutical ingredient (API) in crystal structure determines its various properties including physical, chemical, thermodynamic, kinetic, spectroscopic, mechanical, and surface properties. A thorough understanding of the relationships between crystal structures and the properties of API is critical in selecting the solid state form which can be manufactured reliably and reproducibly. These properties can also have major impact on formulation processing and drug product properties. This session aims to examine the role of crystal structures in designing and selecting solid state form to obtain optimum drug product. Topics may include design & realization of solid forms & their properties, solid form selection and risk assessment, structure property relationships e.g. hydration/dehydration, physical & chemical stability, compressibility & tabletability, role of solid state form in selection of formulation platform

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2:00 - 2:30pm
178 Harnessing the Power of Structural Data for Solid Form Assessment - in partnership with The Crystal Form Consortium
Dr Ghazala Sadiq, Dr Joanna Stevens, Dr Pablo Martinez-Bulit, Dr Elna Pidcock
CCDC, Cambridge, Cambridgeshire, United Kingdom

2:30 - 3:00pm
503 Training the Next Generation of Crystal Engineers
Heba Abourahma
College of New Jersey, Ewing, NJ, USA

3:30 - 4:00pm
266 Mechanistic Investigations of Solid State Desolvation Processes
JENNIFER A SWIFT
Georgetown University, Washington, DC, USA

4:00 - 4:30pm
146 The importance of crystal structure prediction for developing drug molecules.
Dr. Luca Iuzzolino
Merck & Co., Inc., Rahway, NJ, USA

4.2.2: The Future of Light Sources

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Waterview AB
Tiffany Kinnibrugh

Technological advancements in automation, new protocols and equipment for mail-in and remote access, and brighter sources are enabling new research areas and opportunities for diversity and inclusion. Coupling these advances with machine learning (ML) and artificial intelligence (AI) is impacting both the materials and MX science. This session will provide an overview of the impact that these advances are having on the field of structural sciences now and in the future.

2:00 - 2:30pm
371 Self-driving Multimodal Studies at User Facilities
Phillip M Maffettone1, Daniel B Allan1, Stuart I Campbell1, Matthew R Carbone1, Thomas A Caswell1, Brian L DeCost2, Dmitri Gavrilov1, Marcus D Hanwell1, Howie Joress2, Joshua Lynch1, Bruce Ravel2, Stuart Wilkins1, Jakub Wlodek1, Daniel Olds1
1Brookhaven National Laboratory, Upton, NY, USA. 2National Institute of Standards and Technology, Gaithersburg, MD, USA

2:30 - 3:00pm
277 Improving access and throughput of the MX beamlines at Diamond Light Source, UK
Marco Mazzorana, David Aragao, Neil Paterson, Elliot Nelson, Felicity Bertram, Dave Hall
Diamond Light Source, Didcot, Oxon, United Kingdom

3:30 - 4:00pm
343 New Capabilities of the Structural Science Group Beamlines before and after the APS Upgrade
Wenqian Xu, Saul Lapidus, Lynn Ribaud, Olaf Borkiewicz, Tiffany Kinnibrugh, Andrey Yakovenko, Kevin Beyer, James Weng, Tianyi Li, Kamila Wiaderek, Guy Jennings, Charles Kurtz, Uta Ruett
Argonne National Laboratory, Lemont, IL, USA

4:00 - 4:30pm
107 A perfect liaison: combining microED with PXRD
Johannes Merkelbach, Christian Jandl, Danny Stam, Sebastian Schegk
ELDICO Scientific AG, Villigen, Aargau, Switzerland

4.2.3: Computational techniques for SAS

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Waterview CD
Steve Meisburger, Thomas Weiss

Small-Angle Scattering (SAS) has emerged as a powerful technique for integrating high resolution structural information to visualize complex molecular behaviors in solution. The success of artificial intelligence (AI) and machine learning (ML) for structure prediction has made SAS more important than ever: there is a growing need to provide solution context and validation for predicted structures in a robust and high-throughput fashion. This session highlights new experimental and computational approaches for SAS to meet the challenges and opportunities created by AI & ML, as well as scientific applications of SAS enabled by new computational methods.

2:00 - 2:30pm
317 Conformational changes and flexibility in cobalamin-dependent methionine synthase (MetH) studied by SAXS and Cryo-EM
Maxwell B Watkins1, Haoyue Wang2, Audrey A Burnim2, Nozomi Ando2
1BioCAT/IIT, Argonne, IL, USA. 2Cornell University, Ithaca, NY, USA

2:30 - 3:00pm
251 Structural characterization and targeting of higher-order promoter G-quadruplexes
Dr. Robert C Monsen1, Lynn W DeLeeuw1, Dr. William L Dean1, Dr. Robert D Gray1, Dr. Srinivas Chakravarthy2, Dr. Jesse B Hopkins2, Dr. Jonathan B Chaires1, Dr. John O Trent1
1University of Louisville School of Medicine, Louisville, KY, USA. 2Illinois Institute of Technology, Chicago, IL, USA

3:30 - 4:00pm
171 Fitting High-Resolution Electron Density Maps from Atomic Models to Solution Scattering Data
Dr. Sarah Chamberlain, Jitendra Singh, Dr. Thomas Grant
University at Buffalo Jacobs School of Medicine & Biomedical Sciences, Buffalo, NY, USA

4:00 - 4:30pm
312 Explicit atom deuterium contrast matching for small angle neutron scattering on biomolecular systems
Alan Hicks1, Paul Abraham1, Wellington Leite1, Qiu Zhang1, Kevin Weiss1, Hugh O'Neill1, Loukas Petridis1, Jeremy C Smith1,2
1Oak Ridge National Laboratory, Oak Ridge, TN, USA. 2The University of Tennessee - Knoxville, Knoxville, TN, USA

4:30 - 5:00pm
262 Multimodal Modeling of Flexible and Conformationally Heterogeneous Molecules
Dr Patrick J Fleming, Professor Karen G Fleming
The Johns Hopkins University, Baltimore, MD, USA

4.2.4: Electron Tomography

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Kent A-C
Devrim Acehan, Lindsey Backman

Typically, when scientists think of structural biology, their minds turn to high-resolution macromolecular structures obtained through methods such as X-ray crystallography and electron microscopy. Although resulting in lower resolution data, electron tomography (ET) provides researchers with the ability to obtain structural and spatial information for macromolecules, within the context of cellular environments. This session will highlight specimen preparation, data collection, data processing, and analysis developments that are enabling researchers to push the current limits for ET. In addition, you will hear stories about new applications for how ET is combined with light microscopy, structural, and biochemical methods to gain insights into how various macromolecules function within cells.

2:00 - 2:30pm
254 Towards the Visual Proteomics of C. reinhardtii using High-throughput Collaborative in situ Cryo-ET
Dr. Abhay Kotecha
Thermo Fisher Scientific, Eindhoven, North Brbant, Netherlands

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2:30 - 3:00pm
337 TomoDRGN: resolving structural heterogeneity in situ
Professor Joseph Davis1, Mr. Barrett Powell1, Professor Shyamal Mosalaganti2
1Massachusetts Institute of Technology, Cambridge, MA, USA. 2The University of Michigan Life Sciences Institute, Ann Arbor, MI, USA

3:30 - 4:00pm
368 Periodic arrangement of translational machinery within cardiac muscle fibers
Shyamal Mosalaganti1, Andre Schwarz2, Shruti Hemanna3, Joerg Heineke3, Martin Beck4
1University of Michigan, Ann Arbor, Michigan, USA. 2Max Planck Institute for Brain Research, Frankfurt, Hessen, Germany. 3University of Heidelberg, Mannheim, BW, Germany. 4Max Planck Institute of Biophysics, Frankfurt, Hessen, Germany

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4:00 - 4:30pm
235 Beyond MicroED: Ab Initio Crystal Structures Using 4D-STEM
Ambarneil Saha1, Alexander Pattison2, Matthew Mecklenburg1, Aaron Brewster2, Peter Ercius2, Jose A Rodriguez1
1University of California, Los Angeles, California, USA. 2Lawrence Berkeley National Laboratory, Berkeley, California, USA

4:30 - 5:00pm
273 Leveraging Cryo-Electron Microscopy to Reshape Drug Discovery Landscape
Surajit Banerjee

Thermo Fisher Scientific, Hillsboro, OR, USA

4.2.5: Microcrystal Electron Diffraction of Proteins (MicroED)

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Laurel CD
Sarah Bowman, Brent Nannenga

Taking advantage of vanishingly small crystals and electron microscopy instrumentation in diffraction mode, microcrystal electron diffraction (MicroED) is a rapidly growing method for structure determination of biological macromolecules. This session will focus on 1) new macromolecular structures determined using MicroED and 2) methodological advances in MicroED techniques.

2:00 - 2:30pm
268 Seeing is believing: Visualizing submicron crystals as a first step towards direct protein sample preparation for microED experiments
Miranda L Lynch, Elizabeth Snell, Sarah EJ Bowman
Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA

2:30 - 3:00pm
363 Structural studies of GPCRs with MicroED
Anna Shiriaeva
UCLA, Los Angeles, CA, USA

3:30 - 3:50pm
239 Design and implementation of suspended drop crystallization
Mr Cody Gillman, Dr Michael Martynowycz, Dr William J Nicolas, Dr Tamir Gonen
University of California, Los Angeles, Los Angeles, CA, USA

3:50 - 4:10pm
303 A Complete Micro-Electron Diffraction (MicroED) Solution for Fast Structure Determination of Macromolecules and Small Molecules
Dr. Jonathan R Herrmann1, Dr. Natalie Young1, Dr. Abhay Kotecha2
1Thermo Fisher Scientific, Hillsboro, OR, USA. 2Thermo Fisher Scientific, Eindhoven, NB, Netherlands

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4:10 - 4:30pm
203 An automated approach to MicroED enables structure determination of complex samples.
Dr Johan Unge1, Dr Jieye Lin1, Dr Sara J Weaver1, Dr Callie Saeher1, Prof. Tamir Gonen1,2,3
1Department of Biological Chemistry, Los Angeles, CA, USA. 2Howard Hughes Medical Institute, University of California, Los Angeles, CA, USA. 3Department of Physiology, University of California, Los Angeles, CA, USA

4:30 - 4:50pm
296 Novel Macrocyclic Antibiotic structure targeting BamA against Gram-negative Pathogens

Dr Byung-Kuk Yoo1, Dr Ryan Miller2, Dr Sarah Bowman3, Dr Douglas Rees4, Dr Kim Lewis2
1Thermo Fisher Scientific, Kenilworth, NJ, USA. 2Antimicrobial Discovery Center, Department of Biology, Northeastern University, Boston, MA, USA. 3National Crystallization Center, Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA. 4Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, USA

4.2.6: General Interest III

2:00 - 5:00pm Tuesday, 11th July, 2023
Locations Laurel AB
Karen Glass, Timothy Mueser

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

2:00 - 2:30pm
134 RS-MTDock: MovableType ligand docking method using X-ray/Cryo-EM experimental density and integrated QM/MM realspace refinement for drug design
Dr. Oleg Y Borbulevych, Dr. Lance M Westerhoff
QuantumBio Inc., State College, PA, USA

2:30 - 3:00pm
133 Atomic-level determinants of SARS-CoV-2 spike trafficking during infection and vaccination
Dr Debajit Dey1, Dr Suruchi Singh1, Dr Enya Qing2, Dr Yanan He3, Dr Yihong Chen3, Dr Benjamin Jennings4, Mr Whitaker Cohn5, Dr Lokesh Gakhar6,7,8, Dr Nicholas J Schnicker7, Dr Brian G Pierce9,3,10, Prof Julian P Whitelegge5,11,12, Dr Balraj Doray4, Prof John P Orban13,3, Prof Tom Gallagher2, Dr S Saif Hasan1,10,14
1Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, Baltimore, MD, USA. 2Department of Microbiology and Immunology, Loyola University Chicago, Maywood, IL, USA. 3W. M. Keck Laboratory for Structural Biology, University of Maryland Institute for Bioscience and Biotechnology Research, Rockville, MD, USA. 4Department of Internal Medicine, Hematology Division, Washington University School of Medicine, St Louis, MO, USA. 5Pasarow Mass Spectrometry Laboratory, The Jane and Terry Semel Institute for Neuroscience and Human Behavior, David Geffen School of Medicine, University of California, Los Angeles, CA, USA. 6Department of Biochemistry, Carver College of Medicine, University of Iowa, Iowa City, IA, USA. 7Protein and Crystallography Facility, Carver College of Medicine, University of Iowa, Iowa City, IA, USA. 8PAQ Therapeutics, Cambridge, MA, USA. 9Department of Cell Biology and Molecular Genetics, University of Maryland, College Park, MD, USA. 10University of Maryland Marlene and Stewart Greenebaum Cancer Center, University of Maryland Medical Center, Baltimore, MD, USA. 11Molecular Biology Institute, University of California, Los Angeles, CA, USA. 12Jonsson Comprehensive Cancer Center, University of California, Los Angeles, CA, USA. 13Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, USA. 14Center for Biomolecular Therapeutics, University of Maryland School of Medicine, Rockville, MD, USA

3:30 - 4:00pm
120 Current status of Pt-based 1D solids: structures, photoluminescence and electrical conductivity.
Prof. Nikolay N. Gerasimchuk
Missouri State University, Springfield, MO, USA

4:00 - 4:30pm
325 Improvements to Time-Resolved Structural Study using Mix-and-Quench Crystallography
John A Indergaard1, Dr. Matthew McLeod1, Ash Mahmood1,2, Dr. Robert Thorne1
1Cornell University, Ithaca, NY, USA. 2University of Waterloo, Waterloo, Ontario, Canada

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4:30 - 5:00pm
152 Understanding how the Pel polysaccharide is modified for use in the Pseudomonas aeruginosa biofilm
Jaime C. Van Loon1,2, Dr. François Le Mauff3,4,5, Dr. Elena N. Kitova6, Stephanie Gilbert2, Mario A. Vargas2, Dr. Erum Razvi1,2, Dr. John S. Klassen6, Dr. Donald C. Sheppard3,4,5, Dr. P. Lynne Howell1,2
1University of Toronto, Toronto, Ontario, Canada. 2The Hospital for Sick Children, Toronto, Ontario, Canada. 3McGill University, Montreal, Québec, Canada. 4Research Institute of the McGill University Health Centre, Montreal, Québec, Canada. 5McGill Interdisciplinary Initiative in Infection and Immunity, Montreal, Québec, Canada. 6University of Alberta, Edmonton, Alberta, Canada