

Agenda for Pittsburgh Diffraction Conference hosted at the Advanced Photon Source (APS)



Time	Lower Gallery Bldg 402	E1100/E1200 Bldg 402
Sun, Oct 2, 1 pm	Registration	
Sun, Oct 2, 2 pm	Opening / welcome	
Sun, Oct 2, 2:30 pm	"Welcome to APS" Laurent Chapon, Director of APS	
Sun, Oct 2, 3:30 pm	Break	
Sun, Oct 2, 4 pm	Session 1A Upgrade plans for biology / MX beamlines Chair: Zhongmin Jin	Session 1B Upgrade plans for diffraction beamlines for chemistry and material science" Chair: Angus Wilkinson
Sun, Oct 2, 4:00 pm	Dean Haeffner (ANL)	Peter Kenesei (ANL)
Sun, Oct 2, 4:25 pm	Robert Fischetti (ANL)	Uta Ruett (ANL)
Sun, Oct 2, 4:50 pm	Karolina Michalska (ANL)	Jason Benedict (Buffalo)
Sun, Oct 2, 5:15 pm	Thomas Irving (IIT)	Zulu Maddury Somayazulu (ANL)
Sun, Oct 2, 5:40 pm	Poster Session / Vendors / Reception	
Sun, Oct 2, 7 pm	End of 1 st Day	



Mon, Oct 3, 8:30 am	Session 2 A “CryoEM microcrystal diffraction: a new tool for the structural biologist” Chair: Brent Nannenga	Session 2B, “New opportunities: coherent x-ray beam” Chair: Stephan Hruszkewycz
Mon, Oct 3, 8:30 am	Tamir Gonen (UCLA)	Yanwen Sun (SLAC)
Mon, Oct 3, 8:55 am	Emma Danelius (UCLA)	Dina Sheyfer (ANL)
Mon, Oct 3, 9:20 am	Brent Nannenga (ASU)	Ross Harder (ANL)
Mon, Oct 3, 9:45 am		Stephan Hruszkewycz (ANL)
Mon, Oct 3, 10:10 am	Collaboration break / Vendors	
Mon, Oct 3, 10:30 am	Session 3A “AI and crystallography” Chair: James Holton	Session 3B “Automation and autonomous experiments” Chair: Kevin Stone
Mon, Oct 3, 10:30 am	Sabine Hollatz (SLAC)	Daniel Olds (BNL)
Mon, Oct 3, 10:55 am	Stephanie Wankowicz (UCSF)	Suchismita Sarker (CHESS)
Mon, Oct 3, 11:20 am	Zheng-Qing Fu (UGA/SER-CAT)	Chris Tassone (SLAC)
Mon, Oct 3, 11:45 pm		Joe Strzalka (ANL)
Mon, Oct 3, 12:10 pm	Lunch / APS tour / Vendors / Poster	
Mon, Oct 3, 12:15 pm	Joe Ferrara (Rigaku)	Vendor 2
Mon, Oct 3, 12:35 pm	Vendor 3	Joern Lange (X-spectrum)
Mon, Oct 3, 12:55 pm	Joyce Frank “MiTeGen Solution for SSX”	Pascal Hofer (DECTRIS)
Mon, Oct 3, 1:30 pm	Session 4 A “MX and Room Temperature Crystallography Studies” Chair: Aina Cohen and Leighton Coates	Session 4B “PDF in bulk and thin films” Chair: Olaf Borkiewicz
Mon, Oct 3, 1:30 pm	Simone Brixius-Anderko (Pitt)	Karena Chapman (SBU)
Mon, Oct 3, 1:55 pm	Marcus Fischer (StJude)	Yaohua Liu (ORNL)
Mon, Oct 3, 2:20 pm	Silvia Russi (SLAC)	Ann-Christin Dippel (DESY)
Mon, Oct 3, 2:55 pm		Marc Michel (VT)
Mon, Oct 3, 3:10 pm	Collaboration break / Vendors	
Mon, Oct 3, 3:30 pm	Session 5 A Time-Resolved Structural Biology at the XFEL and Synchrotron Chair: Aina Cohen and Crissy Tarver	Session 5B “Synergies TEM, X-rays, Neutrons” Chair: Cora Lind-Kovacs
Mon, Oct 3, 3:30 pm	Kevin Dalton (Harvard)	Efrain Rodriguez (UMD)
Mon, Oct 3, 3:55 pm	Mark Wilson (UNL)	Nestor Zaluzec (ANL)
Mon, Oct 3, 4:20 pm	Guillermo Calero (Pitt)	Keith Taddei (ORNL)
Mon, Oct 3, 4:45 pm		Ashfia Huq (SNL)
Mon, Oct 3, 5:10 pm	Poster / Vendor	
Mon, Oct 3, 6:30 pm	Banquet and Sidhu Award Presentation Michael Martynowycz Determining membrane protein structures using microcrystal electron diffraction	
Mon, Oct 3, 10 pm	End of 2 nd Day	

Tue, Oct 4, 8:30 am	Session 6 A “The role of the APS in understanding Covid structure-function” Chair: Bob Fischetti	Session 6B “In situ and operando structural science for clean energy” Chair: Andrey Yakovenko
Tue, Oct 4, 8:30 am	Andrzej Joachimiak (ANL)	Julia Oktawiec (NU)
Tue, Oct 4, 8:55 am	Meng Juan (TRSI)	Stephan Rosenkranz (ANL)
Tue, Oct 4, 9:20 am	Karen Anderson (Yale)	Tom Runcevski (SMU)
Tue, Oct 4, 9:45 am	Roy Mariuzza (UMD)	Tim Fister (ANL)
Tue, Oct 4, 10:10 am	Collaboration break / Vendors	
Tue, Oct 4, 10:30 am	Awards and Business Meeting Poster awards Next conference	
Tue, Oct 4, 11:30 am	Lunch / ALCF Tour/ Vendor/ Poster	
Tue, Oct 4, 11:45 am	Vendor 7	Vendor 8
Tue, Oct 4, 12:05 pm	Vendor 9	Vendor 10
Tue, Oct 4, 12:25 am	Vendor 11	Vendor 12
Tue, Oct 4, 1:30 pm	Outlook into the Future James Holton (LBNL) TBA Rajeev Assary (ANL) “AI- assisted Materials Discovery”	
Tue, Oct 4, 3:00 pm	End of Conference	

School on XPD and PDF Analysis on Wednesday, October 5

8:30 – 9:30 am	Introductory Talks	
9:30 – 12:00 pm	Hands on Training XPD	Hands on Training PDF
12:00 pm – 1:00 pm	Lunch Break	
1:00 pm – 3:00 pm	Hands on Training XRD	Hands on Training PDF

Session	Speaker	Title
1A	Dean Haeffner (ANL)	"Overview of the APS-U Upgrade from a Beamline Perspective"
1A	Robert Fischetti (ANL)	"Structural Biology with the APS-U"
1A	Karolina Michalska (ANL)	"eBERlight – a virtual facility for biological and environmental science"
1A	Thomas Irving (IIT)	"Current Capabilities and Planned Upgrades to the BioCAT Beamline 18ID"
1B	Peter Kenesei (ANL)	"Engineering Materials Science"
1B	Uta Ruett (ANL)	"Capabilities of the "Structural Science (SRS)" beamlines after the upgrade of the APS"
1B	Jason Benedict (Buffalo)	
1B	Maddury Somayazulu (ANL)	"HPCAT upgrade plans"
2A	Tamir Gonen (UCLA)	"Quo Vadis MicroED "
2A	Emma Danelius (UCLA)	"Structural investigation of protoglobins using MicroED "
2A	Brent Nannenga (ASU)	"Small molecule structure determination and analysis by MicroED"
2B	Yanwen Sun (SLAC)	"Ultrafast x-ray photon correlation spectroscopy at the Linac Coherent Light Source"
2B	Dina Sheyfer (ANL)	"Coherent X-ray methods and recent advantages in 3D Laue microscopy"
2B	Ross Harder (ANL)	"Bragg Coherent Diffraction Imaging at the Advanced Photon Source"
2B	Stephan Hruszkewycz (ANL)	
3A	Sabine Hollatz (SLAC)	"Machine Learning for Scoring Diffraction Patterns"
3A	Stephanie Wankowicz (UCSF)	"Leveraging machine learning to detect heterogeneous features from diffraction data"
3A	Zheng-Qing Fu (UGA/SER-CAT)	"How AlphaFold2 can help in structure and function research?"
3B	Daniel Olds (BNL)	"Teaching Robots Beamline Science—How Automation and AI is Accelerating Research at Light Sources"
3B	Suchismita Sarker (CHESS)	"ML-guided high-throughput experimentation for material design and discovery"
3B	Chris Tassone (SLAC)	"SMASH-ML: Solving Materials and Structures through Simple Heuristics and Machine Learning"
3B	Joe Strzalka (ANL)	"Automating Sample Handling for Grazing-Incidence X-ray Scattering Experiments"
4A	Simone Brixius-Anderko (Pitt)	"Targeting aldosterone biosynthesis for the treatment of resistant hypertension"
4A	Marcus Fischer (StJude)	"Impact of temperature on ligand binding and discovery"
4A	Silvia Russi (SLAC)	"New Remote Access Program for Elevated-Temperature and Humidity-Controlled Experiments at SSRL"
4B	Karena Chapman (SBU)	
4B	Yaohua Liu (ORNL)	"PIONEER: single-crystal neutron diffractometer for small samples at the Second Target Station"
4B	Ann-Christin Dippel (DESY)	"PDF of thin film systems: new insights from advanced x-ray total scattering techniques"
4B	Marc Michel (VT)	"New Approaches for Unraveling Crystallization Pathways in Geochemical Systems"
5A	Kevin Dalton (Harvard)	"Variational inference to estimate structure factors from unconventional diffraction experiments"
5A	Mark Wilson (UNL)	"Serial Crystallographic Approaches to Understanding Enzyme Mechanism"
5A	Guillermo Calero (Pitt)	"Towards Molecular Movies of Enzyme Catalysis"
5B	Efrain Rodriguez (UMD)	"Solid state reactions on the beamline, what we gain by peering into the 'black box'"
5B	Nestor Zaluzec (ANL)	"Computationally Mediated Diffraction and Imaging in the Argonne PicoProbe Electron Optical Beam Line"
5B	Keith Taddei (ORNL)	"Hydrogen superconductivity's 'hidden variable' in a quasi-1-D candidate spin triplet superconductor"
5B	Ashfia Huq (SNL)	"X-ray and Neutron Diffraction: Which One, When and Why?"
6A	Andrzej Joachimiak (ANL)	
6A	Meng Juan (TRSI)	"A comprehensive epitope map of the SARS-CoV-2 spike protein"
6A	Karen Anderson (Yale)	"Structure-based and Comp. Design of Novel SARS-CoV-2 Protease Inhibitors as Promising Preclinical Candidates"
6A	Roy Mariuzza (UMD)	"Structural Basis for T Cell Recognition of SARS-CoV-2"
6B	Julia Oktawiec (NU)	
6B	Stephan Rosenkranz (ANL)	
6B	Tom Runcevski (SMU)	"In situ Crystallization of Model Minerals on Titan, Saturn's Moon"
6B	Tim Fister (ANL)	"Multiscale characterization of lead acid batteries using x-ray diffraction"