

A banner for the 2021 APS/CNM Users Meeting. The text "2021 APS/CNM USERS MEETING" is displayed in white, bold, sans-serif font against a dark background with a purple and orange light flare effect.

2021 APS/CNM USERS MEETING

APS / CNM 2021 Users Meeting

May 3-7, 2021 and May 10-14, 2021

The 2021 APS/CNM Users Meeting will gather scientists and engineers from diverse fields of research from around the globe to discuss cutting-edge, mission-driven research. The event will feature plenary sessions, workshops and courses, a poster session, and vendor expo.

The entire program will be offered virtually.

ORGANIZING COMMITTEE

A. Jean-Luc Ayitou, Illinois Institute of Technology, Vice-Chair, CNM Users Executive Committee

Lynnean Celmer, CPA, Event Planner

Jacqueline Cole, Cavendish Laboratory, University of Cambridge, Chair, CNM Users Executive Committee

Zou Finrock, Canadian Light Source, Vice-Chair, APS User Organization Steering Committee

Jacki Flood, APS, Lead User Facility MUA Administrator

Katie Gregar, CNM, Associate Director, User Programs & Operations

Kim Toerpe, APS, User Office Administrator

Constance Vanni, APS, Assistant User Program Manager

Fan Zhang, National Institute of Standards and Technology, Chair, APS User Organization Steering Committee

APS/CNM Users Meeting Agenda

MONDAY, MAY 3

APS WK#1: Ultrafast X-ray Techniques for Monitoring Dynamic Structural and Electronic Responses at the Nanoscale

CNM WK#2: Collaborations Opportunities for Industry with CNM

TUESDAY, MAY 4

APS WK#1: Ultrafast X-ray Techniques for Monitoring Dynamic Structural and Electronic Responses at the Nanoscale

Joint APS/CNM WK#3: Interpreting Hierarchical Data at Nanocenters and X-ray User Facilities

WEDNESDAY, MAY 5

APS Training #4: A Tutorial Workshop on XPCS for Probing Dynamics in Soft and Hard Matter

Joint APS/CNM WK#5: Applications of AI/ML to Real-time Multi-modal Analysis at Synchrotron Light Sources and Electron Microscopes

CNM Short Course A: Thin Film Deposition

THURSDAY, MAY 6

APS Training #4: A Tutorial Workshop on XPCS for Probing Dynamics in Soft and Hard Matter

Joint APS/CNM WK#5: Applications of AI/ML to Real-time Multi-modal Analysis at Synchrotron Light Sources and Electron Microscopes

APS Training #6: Dynamic X-ray Crystallography

FRIDAY, MAY 7

APS WK#7: Wide-angle X-ray Photon Correlation Spectroscopy and Application of Speckle Spatio-temporal Correlation in Materials

MONDAY, MAY 10

Combined APS/CNM Plenary Session

APS Plenary Session

CNM Plenary Session

TUESDAY, MAY 11

Joint APS/CNM WK#8: Dynamics in Soft Matter with Emphasis on Complex Fluids

APS WK#9: Advances in COVID-19 Prevention and Treatment Enabled by Structural Biology Research

Special Session: APS Upgrade Q&A

Poster Session

WEDNESDAY, MAY 12

Joint APS/CNM WK#8: Dynamics in Soft Matter with Emphasis on Complex Fluids

APS WK#9: Advances in COVID-19 Prevention and Treatment Enabled by Structural Biology Research

THURSDAY, MAY 13

CNM WK#11: Hybrid Quantum Systems

APS WK#12: Multi-scale X-ray Fluorescence Microscopy Imaging Using Multiple APS Beamlines

APS WK#13: Feedback on Remote and Collaborative Access at the APS – Future Plans

FRIDAY, MAY 14

CNM WK#11: Hybrid Quantum Systems

APS WK#12: Multi-scale X-ray Fluorescence Microscopy Imaging Using Multiple APS Beamlines

APS Workshop #1: Ultrafast X-ray Techniques for Monitoring Dynamic Structural and Electronic Responses at Nanoscale

Organizers: Burak Guzelturk and Donald A. Walko

Interconversion of energy between light, electricity, and heat is at the heart of many important technologies such as optoelectronics, photocatalysis, and thermoelectrics. Developing next-generation devices reaching thermodynamic efficiency limits requires developing a deeper understanding of energy conversion processes at the nanoscale as well as the ability to manipulate these processes on demand. To this end, it is important to realize techniques that can track evolution of energy conversion and transport in nanostructured materials with high temporal and spatial resolution – however this has proven challenging using existing conventional methods.

In this workshop, we will bring together researchers from different disciplines investigating energy conversion dynamics using materials that are either intrinsically nanosized (quantum dots, nanowires, etc.) or have heterogeneities at the nanoscale (e.g., halide perovskites). Particular attention will be paid to measurement techniques that will benefit from the APS-U, such as picosecond pair-distribution function (TR-PDF) and time-resolved nanoprobe x-ray microscopy, via the improvements in high-energy flux and brightness, respectively. We will further discuss potential needs to resolve picosecond thermal and electronic dynamics in nanostructured materials.

Monday, May 3, Morning

- 9:15 – 9:30 Burak Guzelturk (Advanced Photon Source, Argonne National Laboratory)
Introduction and Welcome
- 9:30 – 10:00 Xiaoyi Zhang (Advanced Photon Source, Argonne National Laboratory)
Time-resolved Research Group Capabilities
- 10:00 – 10:30 Aaron Lindenberg (Stanford University, SLAC)
Ultrafast Structural Deformations in the Hybrid Perovskites
- 10:30 – 10:45 Break
- 10:45 – 11:15 Ian Robinson (Brookhaven National Laboratory)
Time-resolved Powder Diffraction Study of the Melting of Palladium
- 11:15 – 11:45 Martin Holt (Center for Nanoscale Materials, Argonne National Laboratory)
Nanoscale Imaging of Structure and Dynamics through Time-resolved Hard X-ray Diffraction Microscopy
- 11:45 – 12:00 Youngjun Ahn (University of Michigan)
Nanoscale Ultrafast Imaging of Photoinduced Structural Phase Transition in FeRh by X-ray Diffraction Microscopy
- 12:00 Dismissal

Tuesday, May 4, Morning

- 9:15 – 9:45 Andrej Singer (Cornell University)
Control of Phonon Dynamics near a Magnetic Order Critical Point
- 9:45 – 10:15 Naomi Ginsberg (University of California, Berkeley)
Optical Transient Microscopy to Track Energy Carriers
- 10:15 – 10:30 Alexandra Brumberg (Northwestern University)
Anisotropic Transient Disorder of Colloidal, Two-dimensional Semiconductor Nanoplatelets
- 10:30 – 10:45 Break
- 10:45 – 11:15 Jenny Lockard (Rutgers University)
Time-resolved X-ray Spectroscopy Studies of Long-lived Photoinduced Charge Separation in Redox-active Metal Organic Frameworks
- 11:15 – 11:30 Thomas Rossi (University of Illinois at Urbana-Champaign)
Electronic Effects at the Zn K-edge of Epitaxial ZnO Nanorods Investigated by Time-resolved X-ray Absorption Spectroscopy
- 11:30 – 12:00 All-attendee Discussion Session: Ideas toward Future Time-resolved Capabilities
- 12:00 Workshop Concludes

CNM WK#2: Collaborations Opportunities for Industry Partnering with CNM

Organizer: Anirudha Sumant

The purpose of this workshop is to introduce the wealth of capabilities and expertise available at the Center for Nanoscale Materials (CNM) at Argonne to industrial users, and to make them aware of the various ways that industry can collaborate with CNM staff scientists towards building a mutually beneficial partnership.

The Center for Nanoscale Materials at Argonne has expertise and state-of-the-art capabilities in the synthesis, characterization, and fabrication of nano-based systems, along with strong theory/simulation support, that is of great interest to start-up, mid-size and large industries. We recognize that, unlike the academic world, industrial users have distinct requirements, timeframes, research objectives, and sensitivities to intellectual property.

In addition to the facilities at CNM, industries may not be aware of several important DOE sponsored programs including the Chain Reaction Innovations (CRI) program and DOE's Technology Commercialization Program, etc. where industry can actively participate with CNM staff scientists in developing new technologies in the most effective way. This workshop will serve as an introduction to industrial staff about such program details as well as how the CNM user proposal mechanism could be used as a vehicle in building meaningful collaboration with CNM staff scientists. This workshop is expected to provide an excellent platform for industrial users to exchange ideas, foster collaborations with user facilities at Argonne to and embark upon new challenges in nanoscience and nanotechnology.

Monday, May 3, Morning

Session 1: Industry Argonne Collaborations (Session Chair: Anirudha Sumant)

- 9:00 – 9:05 Anirudha Sumant (Center for Nanoscale Materials, Argonne National Laboratory)
Welcome and Introduction
- 9:05 – 9:15 Kawtar Hafidi (Physical Science and Engineering Division, Argonne National Laboratory)
Kickoff Address to Participants
- 9:15 – 9:45 Kamal Soni (Corning Inc.)
Corning-Argonne Collaborations in Nanomaterials: Advancing the Research Frontiers
- 9:45 – 10:15 Nobuyuki Kambe (Phoenix Venture Partners)
Ecosystem to Commercialize Nano-Innovations
- 10:15-10:30 Break

Session 2: CNM Capabilities and Expertise (Session Chair: Katie Carrado Gregar)

- 10:30 – 10:45 Martin Holt (Center for Nanoscale Materials, Electron and X-ray Microscopy Group, Argonne National Laboratory)
The Electron and X-ray Microscopy Group at the Center for Nanoscale Materials
- 10:45 – 11:00 Richard Schaller (Center for Nanoscale Materials, Nanophotonics and Biofunctional Structures Group, Electron and X-ray Microscopy Group, Argonne National Laboratory)
Capabilities of the Nanophotonics and Biofunctional Structures (nPBS) Group in the Center for Nanoscale Materials
- 11:00 – 11:15 Anirudha Sumant (Center for Nanoscale Materials, Nanofabrication and Devices Group, Electron and X-ray Microscopy Group, Argonne National Laboratory)
Capabilities and Expertise of the Nanofabrication and Devices Group at the Center for Nanoscale Materials
- 11:15 – 11:30 Nathan Guisinger (Center for Nanoscale Materials, Quantum and Energy Materials Group, Argonne National Laboratory)
Overview of the Quantum and Energy Materials Group
- 11:30 – 11:45 Subramanian Sankaranarayanan (Center for Nanoscale Materials, Theory and Modeling Group, Argonne National Laboratory)
Theory and Modeling Group at the Center for Nanoscale Materials
- 11:45 – 12:00 Questions to the Groups
- 12:00 – 1:00 Lunch Break

Monday, May 3, Afternoon

Session 3: Working with Argonne/CNM (Session Chair: Anirudha Sumant)

- 1:00 – 1:30 Katie Carrado Gregar (Center for Nanoscale Materials, Argonne National Laboratory)
Successful Partnerships via the Center for Nanoscale Materials User Program
- 1:30 – 2:00 Phil Smith (Business Development, Argonne National Laboratory)
A Partner in Innovation: How to Work with Argonne
- 2:00 – 2:30 Chunguang Jing (EuclidTechLab LLC)
Development of UNCD-based Electron Sources and Beyond: From One-time Opportunity to a Long-term Collaboration with CNM
- 2:30 – 3:00 Harpal Singh (Sentient Science Inc.)
DigitalClone® – Digital Representation to Optimize Design and Maximize Life of a Product

3:00 – 3:15 Break

Session 4: Entrepreneurship Opportunities at Argonne (Session Chair: Yu Kambe)

- 3:15 – 3:45 John Carlisle and Deena Wright (Chain Reaction Innovations, Argonne National Laboratory)
Chain Reaction Innovations: Connecting Entrepreneurs, Argonne, and the Chicago Innovation Ecosystem to Move Science-based Innovations into High Impact Applications
- 3:45 – 4:15 Chad Husko (Iris Light Technologies, Inc. and CRI Fellow)
Commercialization of Optoelectronics at the CNM
- 4:15 – 4:45 Carrol Scarlet (Axion Technologies, LLC and CRI Fellow)
Quantum Randomness on a Chip
- 4:45 – 5:00 Yu Kambe (NanoPattern Technologies) and Anirudha Sumant (Center for Nanoscale Materials, Argonne National Laboratory)
Thanks and Closeout

Joint APS/CNM WK#3: Interpreting Hierarchical Data at Nanocenters and X-ray User Facilities

Organizers: Maria Chan, Mathew Cherukara, Wendy Di, and Yue Cao

Understanding the evolution of materials in situ and under operando conditions is fundamental to the rational design and precise control of material properties and requires concerted experimental and theoretical efforts. The key information about the material evolution is contained in the lattice and electronic structures across hierarchies of relevant length and time scales, and is captured using different electron and x-ray spectroscopy, diffraction and imaging instrumentations at national nano and x-ray user facilities. However, the depth of information contained therein can be hard to fully exploit due to the complex nature of the data using typical approaches to analysis. The goal of this workshop is to initiate a discussion focused on increasing the efficiency and amount of information extracted from hierarchical datasets. To make sense of these experimental observations needs a coherent framework to merge large datasets with rigorous theoretical calculations and modeling to validate the questions at hand.

Recent advancement at DOE nanocenters and x-ray user facilities including the improvement of electron and x-ray source qualities, the use of large two-dimensional detectors, and the development of high throughput data acquisition protocols fueled an explosion of user data approaching TB for a single experiment. Meanwhile, modeling complicated material systems is computationally expensive due to the large number of atoms involved and the small energy difference between different configurations. These new challenges in domain science parallel the rapid progress in high-power computing and artificial intelligence, which provides new opportunities to accelerate the understanding and discovery of materials. The bottleneck is bridging the knowledge gap between the domain experts and computing scientists, and between domain experts with different experimental/theoretical areas of expertise.

This workshop will bring together experts in electron/x-ray diffraction, spectroscopy and imaging, atomic simulations, and computing scientists to focus on the following cross-cutting frontiers, including (1) high-throughput feature extraction from large experimental dataset, and the role of HPC in streamlining the data analysis; (2) coherent interpretation of multiple x-ray and electron measurements as higher dimensional data, with the help of machine learning; (3) formation and validation of hypothesis towards supervised experiments at user facilities.

Tuesday, May 4, Morning

8:30 – 8:35 Welcome

8:35 – 8:50 Ilke Arslan (Center for Nanoscale Materials, Argonne National Laboratory)
Opening Remarks

Session 1

8:50 – 9:20 John Freeland (Advanced Photon Source, Argonne National Laboratory)
Buried by Data: My Experience Struggling with High Volumes of Complex X-ray Data

- 9:20 – 9:50 Wonsuk Cha (Advanced Photon Source, Argonne National Laboratory)
Bragg Coherent Diffractive Imaging at APS-U
- 9:50 – 10:20 Deyu Lu (Brookhaven National Laboratory)
Unraveling Local Chemical Environment from X-ray Absorption Spectroscopy Using Theory and Machine Learning
- 10:20 – 10:30 Break

Session 2

- 10:30 – 11:00 Xijie Wang (SLAC National Accelerator Laboratory)
Beyond Bragg Electron Diffraction: Connecting Electronic and Nuclear Dynamics with MeV-UED
- 11:00 – 11:30 Petro Maksymovych (Oak Ridge National Laboratory)
Navigating Disorder in Superconductors Using Atomic-scale Imaging and Machine Learning
- 11:30 – 12:00 Matthew Brahlek (Oak Ridge National Laboratory)
Crosscutting Synthesis with Advanced X-ray Characterization for a Deeper Understanding into Quantum Materials
- 12:00 – 1:00 Lunch Break

Tuesday, May 4, Afternoon

Session 3

- 1:00 – 1:30 Ian Robinson (Brookhaven National Laboratory)
Data-driven Phasing Algorithms for Bragg Coherent Diffractive Imaging
- 1:30 – 2:00 Jing Tao (Brookhaven National Laboratory)
Concurrent Probing of Both Electron and Lattice Dynamics in CDW 1T-TaSeTe Using MeV UED

Session 4

- 2:00 – 2:30 Jianguo Wen (Center for Nanoscale Materials, Argonne National Laboratory)
Low-dose/High-speed Atomic Resolution TEM Imaging of Structural Dynamics
- 2:30 – 3:00 Daniel Dessau (University of Colorado)
Analysis of ARPES Data in Higher Dimensions
- 3:00 – 3:15 Break

Session 5

- 3:15 – 3:45 Shinjae Yoo (Brookhaven National Laboratory)
Toward Automated In Situ Beamline Analysis and Operation
- 3:45 – 4:15 Daniela Ushizima (Lawrence Berkeley National Laboratory)
Multimodal Multiscale Analysis of Biofuel Plants Using Machine Learning
- 4:15 – 4:45 Discussions
- 5:00 Workshop Adjourns

APS Training #4: A Tutorial Workshop on XPCS for Probing Dynamics in Soft and Hard Matter

Organizers: Eric Defresne, Zhang Jiang, and Qingteng Zhang

X-ray photon correlation spectroscopy (XPCS) measures equilibrium and nonequilibrium dynamics in materials by correlating temporal fluctuations of a coherent speckle pattern. Over the past two decades, XPCS has led to many fundamental discoveries in soft matter (polymers, colloidal suspensions, membranes, proteins) and hard-condensed matter (ferroelectrics, metallic glasses, charge density waves). The APS Upgrade will have a tremendous impact on coherence techniques such as XPCS and will enable dynamics studies from sub-microseconds to hundreds of seconds. A new world-leading XPCS beamline is being constructed as part of APS-U with technical infrastructure to deliver the above science.

One of the major hurdles in XPCS reaching out to a broader scientific user community is the challenges associated with data analysis and interpretation. This training tutorial will cover the various important aspects of XPCS, such as its fundamentals, sample preparation, data analysis and interpretation. Special emphasis will be placed on methods to quantify temporally heterogeneous dynamics which opens up novel scientific capabilities after APS-U. The training will primarily target early career principal investigators, graduate students and postdocs.

The workshop topics include, but are not limited to:

- (1) Introduction to coherent x-ray scattering
- (2) Principles of spatial and temporal correlation techniques
- (3) Experimental considerations and sample environments (Rheo-XPCS, Small Angle XPCS, Wide Angle-XPCS, Grazing Incidence-XPCS)
- (4) Data analysis and software infrastructure
- (5) Application cases: polymers, nanoparticle assemblies, spin-glass, metallic glasses, ferroic thin films, battery materials
- (6) How to apply for an XPCS beam time

Wednesday, May 5, Morning

Focus: XPCS Theory and Applications

- 8:50 – 9:00 Alec Sandy (Advanced Photon Source, Argonne National Laboratory)
Opening Remarks
- 9:00 – 10:00 Laurence Lurio (Northern Illinois University)
Probing Material Dynamics Using X-ray Photon Correlation Spectroscopy
- 10:00 – 10:30 Qingteng Zhang (Advanced Photon Source, Argonne National Laboratory)
Small-angle XPCS
- 10:30 – 11:00 Suresh Narayanan (Advanced Photon Source, Argonne National Laboratory)
Rheology XPCS
- 11:00 – 11:15 Break

- 11:15 – 11:45 Zhang Jiang (Advanced Photon Source, Argonne National Laboratory)
Grazing-incidence XPCS
- 11:45 – 12:15 Eric Dufresne (Advanced Photon Source, Argonne National Laboratory)
Wide-angle XPCS
- 12:15 – 12:30 Joseph Strzalka (Advanced Photon Source, Argonne National Laboratory)
Beam Time Application
- 12:30 – 12:45 Qingteng Zhang (Advanced Photon Source, Argonne National Laboratory)
Preparation for Day 2
- 12:45 – 1:00 *Q&A*

Thursday, May 6, Morning

Focus: Hands-on Data Analysis and Visualization

- 9:00 – 10:00 Qingteng Zhang (Advanced Photon Source, Argonne National Laboratory)
Virtual Beam Time Tour
- 10:00 – 11:00 Suresh Narayanan (Advanced Photon Source, Argonne National Laboratory)
Data Flow and Analysis
- 11:00 – 11:15 Break
- 11:15 – 12:00 Qingteng Zhang (Advanced Photon Source, Argonne National Laboratory)
Hands-on Data Visualization
- 12:00 – 12:30 *Q&A and Closing Remarks*

Joint APS/CNM WK#5: Applications of AI/ML to Real-time Multi-modal Analysis at Synchrotron Light Sources and Electron Microscopes

Organizers: Mathew Cherukara, Subramanian Sankaranarayanan, Nicholas Schwarz, and Chengjun Sun

The APS and CNM are in the position to help solve some of the most challenging and novel scientific questions facing the energy needs of the nation. The design of new materials to manipulate classical and quantum information with high fidelity and ultralow power consumption, enabling systems for efficient energy storage, transportation, and conversion that will drive the emerging economy based on renewable energy are just a few examples. Addressing these scientific opportunities will be aided by the intrinsic capabilities of APS-U era facilities along with new measurement techniques and technological advances in detectors.

These advances in sources and detectors (x-ray and electron) will result in orders of magnitude higher data rates and increased complexity from multi-modal data streams. Conventional data processing and analysis methodologies become infeasible in the face of such large and varied data streams. The use of AI/ML methods is becoming indispensable for real-time multi-modal analysis at advanced synchrotron light sources and in electron microscopes. This workshop is organized to discuss the state-of-the-art and potential of AI/ML for real-time multi-modal data processing and analysis. It provides an opportunity for academics, laboratory and facility staff, researchers, and students from x-ray and electron characterization communities to exchange ideas and think creatively about new methods for multi-modal characterization and experimentation.

Wednesday, May 5, Morning

8:50 – 9:00 Welcome Day 1

Session 1

9:00 – 9:30 Prasanna Balaprakash (Argonne National Laboratory)
Neuromodulated Neural Architectures with Local Error Signals for Memory-constrained Online Continual Learning

9:30 – 10:00 Maria Chan (Argonne National Laboratory)
Integrating Machine Learning and Theoretical Modeling for X-ray and Electron Data Inversion

10:00 – 10:30 Stephan Hruszkewycz (Materials Science Division, Argonne National Laboratory)
Opportunities for AI/ML to Enable New Materials Science with Coherent X-ray Diffraction

10:30 – 11:00 Break

Session 2

11:00 – 11:30 Wendy Di (Mathematics and Computer Science Division and X-ray Science Division, Argonne National Laboratory)
Multimodal Inverse Problem in Data Science

11:30 – 12:00 Inhui Hwang (Advanced Photon Source, Argonne National Laboratory)
X-ray Emission Data Analysis Software Package Using Unsupervised Machine Learning

12:00 – 12:15 Closeout Discussion for Day 1

Thursday, May 6, Morning

8:50 – 9:00 Welcome Day 2

Session 3

9:00 – 9:30 Bobby Sumpter (Oak Ridge National Laboratory)
Understanding and Controlling the Materials and Chemical World, Atom-by-Atom

9:30 – 10:00 Stephen Whitlam (Molecular Foundry, Lawrence Berkeley National Laboratory)
Learning to Grow: Control of Material Self-assembly Using Evolutionary Reinforcement Learning

10:00 – 10:30 Remi Dingreville (Center for Integrated Nanotechnologies, Sandia National Laboratories)
Decoding Microstructure Statistics from Diffractograms Via Atomistic Simulations and Machine Learning

10:30 – 11:00 Break

Session 4

11:00 – 11:30 Petrus Zwart (Lawrence Berkeley National Laboratory)
Towards High-throughput Autonomous Infrared Spectromicroscopy

11:30 – 12:00 Hemant Sharma (Advanced Photon Source, Argonne National Laboratory)
AI Accelerated Reconstructions for Real-time Analysis of High-energy Diffraction Microscopy Data at APS

12:00 – 12:15 Closeout Discussion for Day 2

CNM Short Course A: Thin Film Deposition

Organizer: Liliana Stan

This course is designed as an introduction to fundamental concepts and operating principles for the deposition of thin films by physical vapor deposition or chemical methods, providing a broad overview of thin film deposition methods including their advantages and limitations.

Understanding that all methods have their specific limitations and involve compromises with respect to process specifics and substrate material helps in determining the methods that are suitable for achieving the expected film properties. Deposition methods that are available at the Center for Nanoscale Materials (CNM) - sputtering, evaporation, ALD, and CVD - will be discussed in more detail.

Wednesday, May 5, Afternoon

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| 1:30 – 1:40 | Liliana Stan (Center for Nanoscale Materials, Argonne National Laboratory)
<i>Thin Films Characteristics and Deposition Methods</i> |
| 1:40 – 2:10 | Liliana Stan (Center for Nanoscale Materials, Argonne National Laboratory)
<i>Sputtering and Evaporation</i> |
| 2:10 – 2:20 | Break/Discussion |
| 2:20 – 3:00 | Liliana Stan (Center for Nanoscale Materials, Argonne National Laboratory)
<i>Atomic Layer Deposition (ALD)</i> |
| 3:00 – 3:20 | David Czaplewski (Center for Nanoscale Materials, Argonne National Laboratory)
<i>Chemical Vapor Deposition (CVD)</i> |
| 3:20 – 3:30 | Discussion |

APS Training #6: Dynamic X-ray Crystallography

Organizers: Robert Henning, David Kissick, and Darren Sherrell

The APS-U will provide a highly brilliant beam ideally suited for serial crystallography methods. In preparation for the new source, GM/CA@APS, SBC, and BioCARS at the APS are hosting this collaborative workshop for user demonstrations in sample preparation, data collection, and data processing for serial millisecond crystallography (SMX). This method has the potential to visualize dynamic processes in macromolecules and to address the substantially faster x-ray damage that will occur with the brighter APS-U beam. Participants will receive demonstrations and training with crystal handling, sample delivery to the x-ray beam, data collection approaches, beamline controls as well as auto- and post-processing and structure determination.

Serial crystallography methods have many advantages: low dose per crystal, room temperature collection, and reduced radiation damage per crystal, allowing the use of small or x-ray sensitive samples and the ability to perform time-resolved measurements. Initially developed at XFELs, serial experiments have been implemented and expanded at synchrotron sources. Advances in SMX experiments are paramount for the APS-U, as this method is expected to flourish with the significant increase in x-ray flux density and a concomitant rise in multi-crystal datasets. Proof-of-principle and groundbreaking experiments using the injection method were conducted by GM/CA@APS and BioCARS, and SBC recently began offering fixed-target collaborative users. GM/CA@APS has worked to advance this method by improving signal-to-noise with tapered beamstops and focusing via compound refractive lenses. SBC has worked on sample preparation, delivery, ease-of-use, and developed collaborations within Argonne, including the supercomputing group, for automatic data analysis and feedback. BioCARS uses Laue crystallography technique for time-resolved studies and has expanded its use to fixed-target serial crystallography compatible with use of short laser pulses for reaction initiation. Experimenters now have access to well-rehearsed methods and free data processing software packages such as CrystFEL and DIALS. Serial crystallography is now feasible at the APS and is becoming routine at these beamlines. Interest in the scientific community is growing for those who have seen that the method can be straightforward.

At GM/CA@APS, participants will receive demonstrations and training with a viscous jet injector, and at SBC, they will gain exposure to the high-speed fixed-target equipment. Users will see demonstrations in methods of sample handling, delivery, and data collection using standard samples provided by the organizers. Participants unfamiliar with the serial techniques will explore approaches to data processing and analysis.

Thursday, May 6, Morning

10:00 – 10:10 David Kissick (Advanced Photon Source, GM/CA, Argonne National Laboratory)
Opening Remarks

- 10:10 – 10:35 Darren A. Sherrell (Advanced Photon Source, SBC-CAT, Argonne National Laboratory)
Serial Crystallography at the APS
- 10:35 – 11:00 Alke Meents (Deutsches Elektronen-Synchrotron, DESY)
Microsecond Time Resolved Fixed-Target Serial Crystallography
- 11:00 – 11:25 Jose Martin Garcia (Instituto de Quimica Fisica Rocasolano, CSIC)
Monochromatic and Pink X-ray Beam Serial Synchrotron Crystallography with Viscous Jets
- 11:25 – 12:00 Mateusz Wilamowski (University of Chicago/Jagiellonian University)
Time-resolved Snapshots of Antibiotic Cleavage by LIMetallo- β -Lactamase
- 12:00 – 1:00 Lunch Break

Thursday, May 6, Afternoon

Demonstrations (subject to change): The afternoon session will take us through experiments at the three organizing beamlines and their capabilities, including sample preparation, handling, delivery, and analysis.

- 1:00 – 1:45 David Kissick (Advanced Photon Source, GM/CA, Argonne National Laboratory)
GM/CA, Sector 23
- 1:45 – 2:30 Darren A. Sherrell (Advanced Photon Source, SBC-CAT, Argonne National Laboratory) and Ryan Chard (Data Science and Learning Division, Argonne National Laboratory)
SBC-CAT, Sector 19
- 2:30 – 3:15 Robert Henning (The University of Chicago)
BioCARS, Sector 14
- 3:15 – 4:00 Closing Remarks and Open Discussion Period
- 4:00 Adjourn

APS WK#7: Wide-angle XPCS and Application of Speckle Spatio-temporal Correlation in Materials

Organizers: Yue Cao and Eric Dufresne

The APS Upgrade beamline 8-ID will bring great, new capabilities for users of wide-angle x-ray photon correlation spectroscopy (XPCS) as well as more than double current available beam time. This workshop aims to attract new users and provide a forum for discussion on the future capabilities of the beamline and guide long term investments.

Friday, May 7, Morning

8:30 – 8:45 Alec Sandy (Advanced Photon Source, Argonne National Laboratory)
Opening and Welcome

Session 1: Facilities Update

8:45 – 9:20 Eric M. Dufresne (Advanced Photon Source, Argonne National Laboratory)
Coming soon

9:20 – 9:55 Beatrice Ruta (European Synchrotron Radiation Facility)
Complex Systems and Coherent X-rays: A Perfect Match

9:55 – 10:05 Break

Session 2: Functional Materials - Metallic Glass

10:05 – 10:40 Jian-Zhong Jiang (Zhejiang University)
Atomic Dynamics in Metallic Glasses by X-ray Photo Correlation Spectroscopy

10:40 – 11:15 Robert Maass (Federal Institute of Materials Research and Testing & University of Illinois at Urbana-Champaign)
Structural Dynamics in Bulk Metallic Glasses: Effects of Mechanical and Thermal Stresses

11:15 – 11:25 Break

Session 3: Ferroelectrics and Quantum Materials – 1

11:25 – 12:00 David Le Bolloc'h (Université Paris-Sud)
Sliding Properties of a Charge Density Wave Driven by a Coherent Deformation That Extends to Several Tens of Micrometers

12:00 – 12:35 Roopali Kukreja (University of California, Davis)
Coherent X-ray Scattering Studies of Electronic Materials

12:35 – 1:35 Lunch Break

Friday, May 7, Afternoon

Session 4: Ferroelectrics and Quantum Materials – 2

- 1:35 – 2:10 Dina Sheyfer (Argonne National Laboratory)
Relaxor Ferroelectrics under Applied Field Studied Via Wide-angle X-ray Photon Correlation Spectroscopy
- 2:10 – 2:45 Paul Evans (University of Wisconsin-Madison)
Coherence, Fluctuations, and Dynamics in Ferroelectric Nanodomains
- 2:45 – 2:55 Break
- 2:55 – 3:30 Mark Dean (Brookhaven National Laboratory)
Coherent X-ray Studies of Charge and Spin Density Wave Pinning in Cuprates and Nickelates
- 3:30 – 4:05 Dillon Fong (Argonne National Laboratory)
X-ray Photon Correlation Spectroscopy Studies of Oxygen Vacancy Dynamics in Complex Oxide Heterostructures
- 4:05 – 4:15 Break

Session 5: Emerging Topics

- 4:15 – 4:50 JT Hastings (University of Kentucky)
Studying Artificial Spin Ices with Soft X-ray Photon Correlation Spectroscopy
- 4:50 – 5:25 Yanwen Sun (Linac Coherent Light Source)
Realizing Accurate On-the-fly Contrast Determination for X-ray Speckle Visibility Spectroscopy

Combined Plenary Session

Monday, May 10, Morning

Session Chair: Fan Zhang (National Institutes of Science and Technology)

- 9:15 – 9:20 Fan Zhang, Chair, APS Users Organization (National Institute of Standards and Technology)
Welcome and Launch of the 2021 APS/CNM Users Meeting
- 9:20 – 9:30 Paul K. Kearns, Laboratory Director (Argonne National Laboratory)
Welcome from the Laboratory
- 9:30 – 9:35 Stephen Streiffer, Deputy Laboratory Director for Science & Technology and Interim Associate Laboratory Director for PSC (Advanced Photon Source, Argonne National Laboratory)
Introduction of Linda Horton
- 9:35 – 10:00 Linda Horton, Associate Director of Science for Basic Energy Sciences (US Department of Energy, Office of Basic Energy Sciences)
The DOE Perspective
- 10:00 – 10:05 Ilke Arslan, Division Director (Center for Nanoscale Materials and the Nanoscience and Technology Division, Argonne National Laboratory)
Introduction of Keynote Speaker Giulia Galli
- 10:05 – 10:45 Keynote Address: Giulia Galli (Pritzker School of Molecular Engineering, The University of Chicago)
The Many Facets of Light-activated Matter: From Energy Sustainability to Quantum Information Science
- 10:45 – 11:00 Break
- 11:00 – 11:20 Stephen Streiffer, Deputy Laboratory Director for Science & Technology and Interim Associate Laboratory Director for PSC (Advanced Photon Source, Argonne National Laboratory)
APS Update
- 11:20 – 11:40 Ilke Arslan, Division Director (Center for Nanoscale Materials and the Nanoscience and Technology Division, Argonne National Laboratory)
CNM Update
- 11:40 Adjourn

APS Plenary Session

Monday, May 10, Afternoon

Session Chair: Zou Finfrock (Canadian Light Source, Science Division)

- 1:25 – 1:35 Zou Finfrock (Canadian Light Source, Science Division)
Welcome
Announcement of the 2021 Gopal K. Shenoy Excellence in Beamline Science Award Winner
- 1:35 – 1:50 Robert Hettel (Advanced Photon Source, Argonne National Laboratory)
APS Upgrade Update
- 1:50 – 2:30 2021 Arthur H. Compton Award Talks
Mark Rivers (Center for Advanced Radiation Sources (CARS), The University of Chicago)
Reflections on 45 Years of Progress in X-ray Detectors and Data Acquisition

Steve Sutton (Center for Advanced Radiation Sources and Department of the Geophysical Sciences, The University of Chicago)
Earth and Planetary Science with the GSECARS X-ray Microprobe
- 2:30 – 3:10 Michael Toney (University of Colorado)
Insights into Ion Transport with Coherent X-rays
- 3:10 – 3:20 Break
- 3:20 – 3:40 Hsinhan (Dave) Tsai (First Solar)
2020 Rosalind Franklin Award Talk
Synchrotron Characterization for Emergent Hybrid Perovskites Materials
- 3:40 – 4:20 Anthony Rollett (Carnegie Mellon University)
High-energy X-ray Microscopy Insights into Additive Manufacturing
- 4:20 – 5:00 Di-Jia Liu (Chemical Sciences & Engineering Division, Argonne National Laboratory and Pritzker School of Molecular Engineering, The University of Chicago)
Developing Next-generation Electrocatalysts for Fuel Cell, Water Splitting, and CO₂ Conversion Applications

CNM Plenary Session

Monday, May 10, Afternoon

Moderator: Jean-Luc Ayitou, Vice-Chair, CNM Users Executive Committee

- 1:30 – 2:15 CNM Keynote Address: Stephen Forrest (University of Michigan Professor of Electrical Engineering & Computer Science, Physics and Materials Science & Engineering)
Organic Heterojunctions: A Platform for Understanding and Controlling the Optical and Electronic Properties of Disordered Materials
- 2:15 – 3:00 Alex Martinson (Materials Science Division, Argonne National Laboratory)
Towards Precision Inorganic Clusters: Sequential Infiltration Synthesis, Atomic Structure and Conductivity
- 3:00 – 3:20 Break
- 3:20 – 3:30 CNM Users Executive Committee
Update from the CNM Users Executive Committee
- 3:30 – 4:30 CNM Users Town Hall
Topics: Input on Future Capabilities; Writing a Successful CNM User Proposal
- 4:30 Adjourn

Joint APS/CNM WK#8: Dynamics in Soft Matter with Emphasis on Complex Fluids (XPCS)

Organizers: Xiao-Min Lin, Suresh Narayanan, and Qingteng Zhang

Soft matter is a class of materials that includes complex fluids such as polymers, liquid crystals, and colloidal suspensions. The presence of hierarchical structures from micrometer to nanometer scales instills these materials with highly unusual structural and dynamical properties. As part of the APS-Upgrade, a world leading x-ray photon correlation spectroscopy (XPCS) beamline dedicated to probing correlations between structure and dynamical fluctuations is being built to leverage the coherence properties of the new source.

The technical capabilities will include but not limited to probing equilibrium and non-equilibrium dynamics in thermally activated systems as well as under applied shear. The phase space covered will range from 1 nm –1000 nm and microseconds to hundreds of seconds. To fully leverage the new capabilities, it is imperative that we need to expand the general user community for XPCS. The proposed workshop will bring together a mixed set of speakers comprising of researchers with established track record in application of XPCS to this area of research, experts in theory and simulation and domain experts to utilize the new capabilities for collectively advancing the understanding of dynamic phenomena in complex fluids.

The goal of the workshop is to build a library of novel XPCS experiments that could be carried out by the domain experts at the conception of the new beamline.

Tuesday, May 11, Morning

9:00 – 9:15 Suresh Narayanan (Advanced Photon Source, Argonne National Laboratory) and Xiao-Min Lin (Center for Nanoscale Materials, Argonne National Laboratory)
Opening Remarks

9:15 – 9:45 Qingteng Zhang (Advanced Photon Source, Argonne National Laboratory)
APS-U SA-XPCS Beamline

Session 1 Chair: Samanvaya Srivastava, University of California, Los Angeles

9:45 – 10:15 Mahesh Mahanthappa (University of Minnesota)
XPCS Analyses of Disordered and Ordered Sphere-forming Diblock Polymer Melts

10:15 – 10:45 Arthi Jayaraman (University of Delaware)
New Computational Methods to Analyze and Interpret Small-angle Scattering Profiles for Polymers and Soft Materials

10:45 – 11:05 Samanvaya Srivastava (University of California, Los Angeles)
Session Discussion

11:05 – 11:20 Break

Session 2 Chair: Jeffrey Richards, Northwestern University

- 11:20 – 11:50 Ryan Poling-Skutvik (University of Rhode Island)
Relating Dynamics of Soft Materials across Nano, Micro, and Mesoscales
- 11:50 – 12:20 Sanat Kumar (Columbia University/Brookhaven National Laboratory)
Dynamic Scattering Techniques to Understand the Unusual Transport Behavior of Grafted Nanoparticle Melts
- 12:20 – 12:50 Michael Hore (Case Western Reserve University)
Polymer Structure and Dynamics in the Corona of Hairy Nanoparticles
- 12:50 – 1:20 Jeffrey Richards (Northwestern University)
Session Discussion
- 1:20 – 1:30 Suresh Narayanan (Advanced Photon Source, Argonne National Laboratory)
Closing Remarks

Wednesday, May 12, Morning

- 9:00 – 9:15 Xiao-Min Lin (Center for Nanoscale Materials, Argonne National Laboratory)
Overview: Rheo-XPCS Capability

Session 1 Chair: Simon Rogers, University of Illinois, Urbana-Champaign

- 9:15 – 9:45 Robert Leheny (Johns Hopkins University)
Connecting Microscopic Dynamics and Rheology of Soft Materials with X-ray Photon Correlation Spectroscopy
- 9:45 – 10:15 Emanuela Del Gado (Georgetown University)
Computational Rheology of Soft Particulate Gels and Jammed Soft Solids: Microscopic Dynamical Processes and Stress Relaxation
- 10:15 – 10:45 Lilian Hsiao (North Carolina State University)
Spatiotemporal Heterogeneities of Gelling Nanoemulsions
- 10:45 – 11:05 Simon Rogers (University of Illinois, Urbana-Champaign)
Session 1 Discussion
- 11:05 – 11:20 Break

Session 2 Chair: James Harden, University of Ottawa

- 11:20 – 11:50 Srinivasa Raghavan (University of Maryland)
Wormlike Micelles and Vesicles in Polar Organic Solvents: Extending Self-assembly to New Systems and Sub-zero Temperatures

- 11:50 – 12:20 Daniel Blair (Georgetown University)
Opto-Rheology of Shear Thickening in Living Active Matter
- 12:20 – 12:50 Lilo Pozzo (University of Washington)
Interfacial Structure and Dynamics in Emulsion Systems from Neutron and X-ray Scattering
- 12:50 – 1:20 James Harden (University of Ottawa)
Session 2 Discussion
- 1:20 – 1:30 Suresh Narayanan (Advanced Photon Source, Argonne National Laboratory) and
Xiao-Min Lin (Center for Nanoscale Materials, Argonne National Laboratory)
Closing Remarks and Plans for Workshop Summary

APS WK9: Advances in COVID-19 Prevention and Treatment Enabled by Structural Biology Research

Organizers: Michael Becker, Karolina Michalska, Kay Perry

The emergence of the novel Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) -- the etiologic agent responsible for the current outbreak of COVID-19 -- mobilized research communities around the world to investigate the virus and the disease at unprecedented speed. To deliver information suitable for the development of vaccines, therapeutics, and diagnostics, researchers representing multiple disciplines and institutions quickly initiated broad collaborations, while DOE user facilities provided unlimited access to resources necessary for this research. As of November 16, 2020, the Advanced Photon Source has been at the forefront of structural biology work, delivering over ~10,000 hours of the beamtime, supporting over 75 teams of researchers, and delivering 95 novel structures.

Broadly, the workshop will present areas where structural biology research, including macromolecular crystallography and cryoelectron microscopy, intersects with in vivo and in silico studies of SARS-CoV-2 and COVID-19. The topics will include (a) viral biology, (b) vaccine, therapeutic, and diagnostic antibody studies, and (c) small-molecule drug discovery as it relates to viral proteases and other viral proteins. In addition, as this year's events emphasize the need for a coordinated, long-term strategy to prevent future pandemics of zoonotic origin, a broader One Health perspective on viral pathogens will be presented.

Tuesday, May 11, Morning

10:00 – 10:05 Kay Perry (NE-CAT, Argonne National Laboratory)

Opening Remarks

10:05 – 10:25 Jason McLellan (University of Texas-Austin)

Structural-based Design of Coronavirus Vaccine Antigens

10:25 – 10:45 Fang Li (University of Minnesota)

Cell Entry Mechanisms of SARS-CoV-2

10:45 – 11:05 Nicholas Hurlburt (Fred Hutchinson Cancer Research Center)

Structural Basis for Potent Neutralization of SARS-CoV-2 and the Role of Antibody Affinity Maturation

11:05 – 11:25 Ian Wilson (The Scripps Research Institute)

Structural Insights into Antibody Responses to SARS-CoV-2 RBD and Escape Mutants

11:25 – 11:45 Q/A, Break

11:45 – 12:05 Pamela Bjorkman (California Institute of Technology)

Neutralizing Antibodies against Coronaviruses

- 12:05 – 12:25 Cheng Zhang (University of Pittsburgh)
Structural Basis for SARS-CoV-2 Neutralization by Potent and Diverse Nanobodies
- 12:25 – 12:45 James Davis (Advanced Leadership Computing Facility, Argonne National Laboratory)
SARS-Cov-2 in the City of Houston: Insights from the Largest Sequencing Effort in the United States in 2020
- 12:45 – 1:05 Q/A, Break
- 1:05 – 1:25 Drew Weissman (University of Pennsylvania)
Nucleoside-modified mRNA-LNP Vaccine for SARS-CoV-2
- 1:25 – 1:45 Andrea Carfi (Moderna)
Development of Moderna COVID-19 Vaccine (mRNA-1273) and Emerging Variants
- 1:45 – 2:05 Erica Saphire (La Jolla Institute for Immunology)
Antibodies Against SARS-CoV-2: A Global Collaboration
- 2:05 – 2:25 Q/A, Roundtable

Wednesday May 12, Morning

- 10:00 – 10:05 Karolina Michalska (SBC-CAT, Argonne National Laboratory)
Opening Remarks
- 10:05 – 10:25 Youngchang Kim (SBC-CAT, Argonne National Laboratory)
Overview of SARS-CoV-2 Proteome Structural Study
- 10:25 – 10:45 Alice Douangamath (Diamond Light Source, UK)
The XChem Platform at Diamond Light Source: Addressing Covid-19 with Fragment-based Drug Discovery
- 10:45 – 11:05 Arvind Ramanathan (Advanced Leadership Computing Facility, Argonne National Laboratory)
Accelerating the Discovery of Therapeutics Using Artificial Intelligence (AI) against COVID-19
- 11:05 – 11:25 Natalie Strynadka (University of British Columbia)
Crystallographic Structure of Wild-type SARS-CoV-2 Main Protease Acyl-enzyme Intermediate with Physiological C-terminal Autoprocessing Site
- 11:25 – 11:45 Q/A, Break
- 11:45 – 12:05 Andrew Mesecar (Purdue University)
Structure-based Design of Broad-spectrum Coronavirus Protease Inhibitors

- 12:05 – 12:25 Robert Hoffman (Pfizer)
*The Discovery of Ketone-based Covalent Inhibitors of Coronavirus 3CL
Proteases for the Potential Treatment of COVID-19*
- 12:25 – 12:45 Yogesh Gupta (University of Texas-San Antonio)
Structural Basis of RNA Cap Modification by SARS-CoV-2: An Inside View
- 12:45 – 1:05 Karla Satchell (Northwestern University)
Structural Insights into SARS-CoV-2 mRNA Capping
- 1:05 – 1:25 Q/A, Break
- 1:25 – 1:45 Haley Dugan (The University of Chicago)
*Memory B Cells Targeting the SARS-CoV-2 Nucleoprotein Display Endemic
Strain Cross-reactivity and Adapt over Time*
- 1:45 – 2:05 Andrzej Joachimiak (SBC-CAT, Argonne National Laboratory)
*Structures of Human Fabs in Complex with N-protein Nucleocapsid RNA Binding
Domain*
- 2:05 – 2:25 Christine Kreuder Johnson (University of California-Davis)
Catalyzing Innovation for Surveillance of Emerging Pandemic Threats
- 2:25 – 2:45 Jonna Mazet (University of California-Davis)
*Transcending Disciplinary Boundaries to Identify and Characterize Risk from
Emerging Viruses before They Become Disease X*
- 2:45 – 3:05 Q/A, Roundtable
- 3:05 – 3:10 Michael Becker (GM/CA@APS, Argonne National Laboratory)
Closing Remarks

CNM WK#11: Hybrid Quantum Systems

Organizers: Xu Han, Dafei Jin, and Xufeng Zhang

Exploring the exotic non-classical phenomena, quantum science promises revolutionary solutions for complicated tasks in computation, communication, and sensing. In the past few years, many remarkable quantum systems have been demonstrated based on a great variety of physical platforms such as spintronics, nanomechanics, superconducting circuits, and quantum optics. To fully exploit the advantages of quantum technology, it has become increasingly pressing to coherently integrate different quantum platforms and establish high-fidelity transduction among them. Such hybrid systems can link distinctively different degrees of freedom and enable distributed quantum computing and sensing as well as quantum information networks at large scales. Nevertheless, developing hybrid quantum systems is a challenging task since it requires efficient interactions between different quantum excitations with extremely low loss and low noise. To achieve this goal, expertise and efforts in multidisciplinary fields have to be combined together.

In this workshop, we aim to bring together researchers working on various hybrid quantum systems to discuss pathways towards addressing the grand challenges in quantum computing and networking. This topic is highly interdisciplinary and involves efforts from a broad community. The diverse background of the speakers and audience will enable in-depth discussions and novel opportunities for QIS research. It will also help create synergies between Argonne/CNM and the worldwide scientific community. With CNM's efforts towards developing a high standard user facility to support the increasing need for quantum infrastructure, this workshop will be a great opportunity for outreach to potential users and obtaining valuable feedback.

Thursday May 13

10:00 – 10:20 Welcome and Introduction

10:20 – 11:05 Andrew Cleland (The University of Chicago)
Superconducting Qubits Entangled with Phonons

11:05 – 11:15 Q & A

11:15 – 12:00 Mark Saffman (University of Wisconsin-Madison)
Neutral Atom Architectures for Hybrid Quantum Processors

12:00 – 12:10 Q & A

12:10 – 1:00 Lunch Break

1:00 – 1:45 Aashish Clerk (The University of Chicago)
Reservoir-engineered Spin Squeezing in Hybrid Systems

1:45 – 1:55 Q & A

- 1:55 – 2:40 John Chiaverini (Massachusetts Institute of Technology Lincoln Laboratory)
Techniques and Technologies for Entanglement Generation in Trapped-ion Quantum Systems
- 2:40 – 2:50 Q & A
- 2:50 – 3:05 Break
- 3:05 – 3:50 Luqiao Liu (Massachusetts Institute of Technology)
Magnon-magnon and Magnon-photon Coupling for Hybrid Quantum Systems
- 3:50 – 4:00 Q & A
- 4:00 – 4:15 Panel Discussion

Friday May 14

- 10:00 – 10:10 Welcome and Introduction
- 10:10 – 10:55 Special Lecture by 2003 Nobel Laureate in Physics
Anthony Leggett (University of Illinois at Urbana-Champaign)
When Is It Better NOT to Know? The Pros and Cons of Ignorance in Physics Research
- 10:55 – 11:05 Q & A
- 11:05 – 11:50 Michael Manfra (Purdue University and Microsoft Quantum Purdue)
Direct Observation of Anyonic Braiding Statistics
- 11:50 – 12:00 Q & A
- 12:00 – 1:00 Lunch Break
- 1:00 – 1:45 Stephen Lyon (Princeton University)
Mobile Electron Spin Qubits on Helium
- 1:45 – 1:55 Q & A
- 1:55 – 2:40 David Schuster (The University of Chicago)
Hybrid Quantum Systems with Superconducting Circuits
- 2:40 – 2:50 Q & A
- 2:50 – 3:05 Break
- 3:05 – 3:50 Michael R. Wasielewski (Northwestern University)
Photogenerated Radical Pairs as Spin Qubits: Exploiting Quantum Entanglement of Electron Spins

3:50 – 4:00 Q & A

4:00 – 4:15 Panel Discussion

4:15 – 4:20 Closing Remarks

APS WK#12: Multi-scale X-ray Fluorescence Microscopy Imaging Using Multiple APS Beamlines

Organizers: Olga Antipova and Lu Xi Li

Biological, chemical, geological, archeological, cultural heritage, and material science samples come with sizes ranging from nanometers to centimeters. The APS facility of Argonne National Laboratory offers a variety of x-ray fluorescence microscopy (XFM) instruments that offer different capabilities including high spatial resolution, flexible sample environment, sensitivity and additional imaging modality. However, most of the instruments have limited resolution range and may have other limitations. In many cases, proper sample preparation, selection of micro- and nanoscopic features, and efficient use of beam time for large-scale samples, such as tissue sections, cathode or catalysis material, and soil aggregates require wider range and options than a single beamline may be able to offer. Fortunately, sequential measurement at beamlines such as 8-BM, 20-ID, 13-ID, 2-ID-D/E, 9-ID-B, and 26-ID with increasing resolution and with sample modification allows for integrated sample measurement, more comprehensive identification of micro features within large samples, and highly improves efficiency of measurements at beamlines with high spatial resolution but slow data collection rate.

This workshop will demonstrate ongoing progress in multi-scale XFM research, including data collection, sample handling and guided modification, as well as developments in sample holders design and visualization software, which all together will significantly improve user experience with multi-beamline imaging. The workshop will familiarize the broader user community with available XFM options at APS and provide ideas for efficient data collection strategy on current APS as well as for upgraded APS beamlines.

Thursday, May 13, Morning

- 8:30 – 8:45 Olga Antipova and Lu Xi Li (Advanced Photon Source, Argonne National Laboratory)
Welcome from the Organizers
- 8:45 – 9:05 Olga Antipova (Advanced Photon Source, Argonne National Laboratory)
X-ray Fluorescence Microscopy at APS Beamlines: Current and Post-APS-U
- 9:05 – 9:25 Tatjana Paunesku (Northwestern University)
Examination of Nanoparticle-transfected HeLa cells Using Multi-scale X-ray Fluorescence Tomography
- 9:25 – 9:45 Martina Ralle (Oregon Health and Science University)
Copper Storage in Vesicles in Mammalian Systems
- 9:45 – 10:10 Joseph Jakes (University of Wisconsin-Madison)
Integrating Multiscale Studies of Chemically Modified Wood
- 10:10 – 10:30 Break

- 10:30 – 10:55 Samuel Webb (Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory)
Multi-scale, Multi-beamline, and Multi-modal Imaging for Life Sciences at SSRL
- 10:55 – 11:10 Elena Rozhkova (Center for Nanoscale Materials, Argonne National Laboratory)
Wireless Optogenetic Modulation of Cortical Neurons Enabled by Radioluminescent Nanoparticles
- 11:10 – 11:30 Stuart Stock (Northwestern University)
Several Scales of the Structural Hierarchy of Mineralized Tissues
- 11:30 – 11:50 Robin Pourzal (Rush University)
Characterization of Intra-cellular Metallic Debris from Total Hip Replacements within Periprosthetic Tissue
- 11:50 – 12:15 Yulia Pushkar (Purdue University)
X-ray Imaging and Spectroscopy of the Brain
- 12:15 Adjourn

Friday, May 14, Morning

- 8:30 – 8:45 Welcome
- 8:45 – 9:05 Lu Xi Li (Advanced Photon Source, Argonne National Laboratory)
In Situ Visualization of the Phase Separation in Amorphous Solid Dispersion
- 9:05 – 9:20 Peng Liu (University of Waterloo)
Algorithm for Attenuation Correction of Confocal Micro-X-ray fluorescence Imaging (CMXRFI) Data and an Application for Redox Mapping
- 9:20 – 9:40 Sarah Wiegold (Center for Nanoscale Materials, Argonne National Laboratory)
Mapping Impurities and Elemental Distribution in Solar Cell Materials
- 9:40 – 10:00 Grace (Yanqi) Luo (Advanced Photon Source, Argonne National Laboratory)
Real-time Image Registration Techniques for Correlative Analysis
- 10:00 – 10:15 Matt Neville (Center for Advanced Radiation Sources, The University of Chicago, Argonne)
Multi-modal X-ray Measurements at the GSECARS Microprobe Beamline APS 13-ID-E
- 10:15 – 10:35 Break
- 10:35 – 11:00 Michael Stuckelberger (Deutsches Elektronen-Synchrotron DESY)
Strategies for Scanning X-Ray Microscopy across Length Scales, Instruments, and Laboratories

- 11:00 – 11:20 Yang Yang (National Light Source II, Brookhaven National Laboratory)
Multimodal X-ray Nano-imaging with Scanning Microscopy: Applications and Data Analysis
- 11:20 – 11:40 Yijin Liu (Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory)
Multi-scale and Multi-modal X-ray Microscopy for Energy Material Science
- 11:40 – 12:00 Tamas Varga (Pacific Northwest National Laboratory)
Phosphorus Solubilization in Trees Promoted by Endosymbiosis
- 12:00 – 12:25 Jorg Maser (Advanced Photon Source, Argonne National Laboratory) and Michael Stuckelberger (Deutsches Elektronen-Synchrotron DESY)
Discussion: Future Directions for Multiscale XFM Imaging
- 12:25 Adjourn

APS WK#13: Feedback on Remote and Collaborative Access at the APS – Future Plans

Organizers: Suresh Narayanan and Alec Sandy

During the pandemic, the APS was faced with the challenge of rapidly expanding the scope of remote beamline (BL) operations for a diverse general user (GU) community. Leveraging work done by macromolecular crystallography (MX) BLs at the APS (especially that done by GM/CA), the APS rose to the challenge and developed remote access tools including web-based access to BL workstations, user access management, and high-performance data distribution. The developments were successfully deployed across a broad suite of non-MX BLs operated by the APS. (MX beamlines had developed this infrastructure previously.)

While the deployed infrastructure has enabled some level of remote operations, the scope of possible experiments has been limited. Looking post pandemic, we are eagerly anticipating the return of GUs to our facility but also see an opportunity to expand upon on pandemic-enabled tools and work practices to grow the scope, complexity, efficiency, and inclusiveness of APS experiments.

This workshop will briefly present the current or imminent status of representative non-MX remote and mail-in operations at the APS, and it will seek input and ideas from the user community to facilitate more broadly collaborative and efficient studies in the future. We are especially seeking feedback around the challenges and possible opportunities in 1) remote access to experiment control, 2) user training, 3) automation, 4) real-time communication, and 5) remote access to data/analysis/visualization tools.

(The workshop is open to all, and we encourage the participation of all but, admittedly, the MX community is and has been far ahead of the non-MX community in this area, so we expect the presentations and discussion will be most pertinent to those outside of the MX community.)

Thursday, May 13, Afternoon

For each subject, we are planning on 15 minutes of presentation and 15 minutes of discussion.

- 1:00 – 1:10 Suresh Narayanan and Alec Sandy (Advanced Photon Source X-ray Science Division, Argonne National Laboratory)
Welcome and Introduction
- 1:10 – 1:40 John Hammonds (Advanced Photon Source X-ray Science Division, Argonne National Laboratory)
Remote Access to Experiment Control
- 1:40 – 2:10 Alexis Quental (Advanced Photon Source X-ray Science Division, Argonne National Laboratory)
User Training

- 2:10 – 2:40 Byeongdu Lee (Advanced Photon Source X-ray Science Division, Argonne National Laboratory)
Automation and Mail-In
- 2:40 – 2:50 Break
- 2:50 – 3:20 Tao Zhou (Center for Nanoscale Materials, Argonne National Laboratory)
Real-time Communication
- 3:20 – 3:50 Ryan Chard (Computing, Environment, and Life Sciences, Data Science and Learning Division, Argonne National Laboratory)
Remote Access to Data/Analysis/Visualization Tools
- 3:50 - 4:00 Suresh Narayanan and Alec Sandy (Advanced Photon Source X-ray Science Division, Argonne National Laboratory)
Wrap-up



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CAEN Technologies Inc. is the North America branch for the family of CAEN companies and products. The CAEN ELS product line offers solutions as digital magnet power supplies, 4-channel digital picoammeters for detector readouts and beamline positioning, as well as various carrier boards and FMC options for MTCA.4. CAEN SpA develops and markets a wide range of high/low voltage power supply systems, as well as front-end/data acquisition modules for nuclear and particle physics detectors.

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OMS Motion (aka Oregon Micro Systems and OMS) has been successfully producing motion control products and services for more than 35 years. Single axis integrated controls with drives as well as complete multi-axis controllers that can coordinate and synchronize up to 10-axes on a single controller. Founded in the early 80's OMS Motion evolved from patented technology that provides advantages in the motion control industry. In the mid 90's OMS was acquired by a publicly traded company with a focus on the medical device markets. OMS continued the motion control business as a subsidiary, while supporting the medical device product development. In early 2017 OMS Motion separated from the public company, under the original leadership of the company's beginnings, and has regained its focus on motion control business. Great effort has gone into the development of the controls and the functionality continuously evolves as more and more unique applications utilize the controllers. OMS products are used in numerous markets worldwide, including semiconductor, lab automation, life sciences, factory automation, large- and small-scale research facilities/projects, and others. OMS controllers are versatile and capable. OMS Motion fosters the philosophy that "there is no success without the customers' success," and they demonstrate this through their commitment to the customers application lifecycle. OMS has earned a strong reputation and is trusted throughout the world.

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Quantum Detectors has provided novel technology to the APS for several years, with the first installation of an Xspress 3 detector readout system in 2014. Since then, several more systems have been installed around the ring enabling higher throughput, wider dynamic range, and faster experiments. As well as advanced detector readout systems we've also installed several MerlinX detectors at the APS. A 55µm energy resolving detector with up to eight thresholds in Colour Mode and employing a Medipix3 ASIC to achieve rates of 1200 Hz in 12-bit mode, MerlinX is a high-performance x-ray imaging detector that requires no supplementary cooling system. Additionally, we have Hexitec: A fully spectroscopic hard x-ray imaging detector which measures the energy and position of every incident photon in the 4-200 keV range. If you'd like to hear how we could provide better usability, enable faster throughput and in some cases offer a completely new mechanism for detection at your beamline, drop us a line to learn more!

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Sydor Technologies

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Sydor Technologies is a leading global provider of advanced x-ray detectors and diagnostic instrumentation for critical science missions and fundamental research. Sydor's commercial engineering expertise transforms cutting-edge technology into complex measurement solutions that generate critical results for advanced high energy density physics experiments occurring at synchrotrons and fusion research facilities around the world. Established in 2004, Sydor Technologies is headquartered in Rochester, NY and supplies systems and support in over 33 countries. For additional information, please visit www.SydorTechnologies.com.

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