2025 APS/CNM Users Meeting Poster Session

May 6, 2025

Posters are indexed by category then author last name.

Categories

Lettering in front of the number indicates facility/program:

- A# – Advanced Photon Source
- C# – Center for Nanoscale Materials
- ESRP# – Exemplary Student Research Program

BIOLOGY

ESRP-1	Glenbrook South High School
A-2	Kissick, David
C-3	Ma, Yin
ESRP-4	Metea Valley High School
ESRP-5	Naperville Central High School
A-6	O’Neal, Jordan
A-7	Patel, Hiral
ESRP-8	St. Charles East High School
ESRP-9	York Community High School

ESRP: Analyzing DNA Sequences from Plastic Degrading Microbes

George Abraham[1], Jones Daniel[1], Roman Fedianovych[1], Yinon Gankin[1], Dominik Grzeszczak[1], Stephanie Jiang[1], Eddie Kim[1], Daniel Kornfeld[1], Alexander Lukas[1], Ryan McMahon[1], Evelyn Neyman[1], Justin Podowski[2], Jeffrey Rylander[1], David Thekkath[1], Jimmy Tsonis[1], Yipei Wang[1], and Isaiah Yang[1]

[1]Glenbrook South High School, Glenview, IL 60026
[2]Data Science and Learning Division, Argonne National Laboratory, Lemont, IL 60439

As plastics are manufactured at an ever-growing rate, and with some requiring more than 500 years to decompose, the accumulation of plastic waste in our environment is of great concern. This experiment aims to study where plastic-degrading microbes are found in our oceans. Using microbial DNA data collected by Tara Ocean, an organization striving to raise awareness of the vitality of our ocean, the gene sequence of over 80 species of plastic degrading microbes were analyzed. The ‘reads/genome’ calculation was performed for each microbe’s genome. A ‘read’ was determined if a 200 base pairs sequence out of the gene’s approximately 1000-3000 base pairs was a match to that of the known microbe’s genome. 246 ocean water samples were analyzed from the six different ocean layers, four biomes, and 19 different ocean locations around the world to study the prevalence of known plastic degrading microbes in these regions.

Returning to Scientific Operations at GM/CA@APS after the APS-Upgrade

David J. Kissick[1], Michael Becker[1], Stephen Corcoran[1], Dale Ferguson[1], Mark Hilgart[1], Oleg Makarov[1], Sergey Stepanov[1], Nagarajan Venugopalan[1], Qingping Xu[1], Shenglan Xu[1], Janet L. Smith[2], and Robert F. Fischetti[1]

[1]GM/CA CAT, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[2]Life Sciences Institute, University of Michigan, Ann Arbor, MI 48109

The Advanced Photon Source (APS) underwent a comprehensive upgrade to replace the original electron storage ring with a new storage ring (APS-U) that increased the x-ray brightness 500 times compared to the APS. The National Institute of General Medical Sciences and National Cancer Institute Structural Biology Facility at the Advanced Photon Source (GM/CA@APS) operates a national user facility for structural biology. During the year-long shutdown for APS-U upgrade, the GM/CA beamlines and infrastructure were almost completely rebuilt to exploit the high brightness of the APS-U. New state-of-the-art focusing optics (mirrors and compound refractive lenses [CRLs]) now provide extremely intense, clean, stable, and rapidly adjustable beam sizes between 1-50 microns. The maximum energy on 23-ID-D was increased to 35 keV to minimize radiation damage. The new high-stability end station table supports both the CRL transfocator and sample environment. The new goniometer allows data collection on crystals down to one micron in size and provide rapid scanning of random or periodic fixed target samples. The recently acquired DECTRIS Eiger2 XE 16M CdTe detector enables high-speed, high-efficiency x-ray detection on our high energy beamline 23-ID-D. The new PyBluIce GUI and beamline control software will enable sophisticated routines such as 3D-rastering, helical and fully automated (unattended) data collection, and routine serial crystallography data collection from fixed target and injector-based sample delivery systems. Technical beamline commissioning with the first x-rays occurred in winter 2024 along with macromolecular crystallography measurements of standard samples. We have begun welcoming users back for scientific commissioning as of spring 2025. Here, we will present the new designs and game-changing opportunities for structural biology research enabled by these small, ultra-intense, high-energy beams.

GM/CA@APS has been funded by the National Cancer Institute (ACB-12002) and the National Institute of General Medical Sciences (AGM-12006, P30GM138396). The Eiger 16M detector was funded by an NIH-Office of Research Infrastructure Programs, High-End Instrumentation Grant (1S10OD012289-01A1). This research used resources of the Advanced Photon Source; a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Improving CryoEM Specimen Preparation and Quality Using Surface Science

Yin Ma[1], Jierui Xia[1], Hiral P. Patel[1], Arjun Balyan[1], and Andrew H. Bond[1]

[1]DeNovX, Chicago, IL 60616

Cryogenic electron microscopy (cryoEM) is widely used for structural studies of non-crystalline and conformationally heterogeneous biological analytes including proteins, complexes, and assemblies in the 50 kDa to 16 MDa range. Ideal specimens require vitrified ice (~1–3 micrometers thick) with sufficient, uniformly dispersed, and randomly oriented particles of the bioanalyte. Unfortunately, sample preparation remains a time-consuming trial and error bottleneck in specimen preparation in which quality is adversely affected by (1) support hydrophobicity resulting in poor bioanalyte incorporation into support film holes, (2) partitioning of bioanalytes to the air-water interface with nonrandom distributions and/or loss of conformational integrity, and (3) orientation bias that may not be discernible until the completion of time-consuming high resolution data collection. Leveraging successes in physical surface energy modification and chemical functionalization for improving protein crystallization outcomes, DeNovX is developing novel cryoEM specimen supports to address these challenges. In collaboration with CNM staff scientists, DeNovX is developing novel cryoEM specimen supports with surface energies, surface chemistries, and hydrophilic/hydrophobic characteristics that are suitable for the different classes of proteins and molecular assemblies studied in cryoEM. This presentation will present our rationale for reproducibly improving cryoEM specimen preparation with examples of the surface science modifications and characterization.

ESRP: The Impact of Arbuscular Mycorrhizal Fungi on the Growth of Herbs in the Presence of Excess Copper

Sahasra Chatakondu[1], Amogh Garde[1], Nitin Gopala[1], Pragya Iyer[1], Rithika Manchala[1], Tiana Prem[1], Sanchit Sidhu[1], Kavya Suravajhela[1], Vanessa Troiani[1], Malgorzata Korbas[2], Qiaoling Jin[2], Antonio Lanzirotti[3], and Matthew Newville[3]

[1]Metea Valley High School, Aurora, IL 60502
[2]eBERlight Group, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[3]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL 60637

Copper (Cu) is a naturally occurring element found in soil and living organisms. As a cofactor for many enzymes involved in photosynthesis, respiration, and antioxidant systems, Cu plays a key role under stress conditions. Cu is also associated with oxidative phosphorylation, protein trafficking, signal regulation, and lipid and iron metabolism in plants [1]. At lower concentrations, Cu is an important micronutrient [2] to plants. However, higher concentrations, such as 100-800 mg kg−1 [3], can have toxic effects on soil microorganisms and hinder the mineralization of essential nutrients, such as phosphorus (P) and nitrogen (N) [4]. Since Cu is present in various forms of electronic technology [5], it could contribute to soil contamination through leaching from discarded electronics. Due to the low mobility of copper, soil contamination and pollution can be long-lasting [6]. Arbuscular Mycorrhizal Fungi (AMF) have been shown to act as organic fertilizers that promote plant growth. AMF has demonstrated the ability to alleviate Cu toxicity in spearmint [2] and other common herbs. In our study, we investigated the effects of AMF inoculations on the growth of two herb species, dill (Anethum graveolens) and thyme (Thymus vulgaris), in Cu-contaminated soil. Throughout the study, we monitored quantitative parameters of the plants post-inoculation, such as growth measurements, as well as qualitative observations including color, texture, and overall form of the plants. We then utilized x-ray fluorescence microscopy at the 13-ID-E beamline of the Advanced Photon Source to compare the distributions of Cu and other essential elements between the roots and leaves of thyme plants grown in the presence or absence of AMF. Our results represent initial steps toward understanding the role of AMF in Cu uptake from soil contaminated by electronic waste.

[1] Nazir, F., Hussain, A., & Fariduddin, Q. (2019). Hydrogen peroxide modulate photosynthesis and antioxidant systems in tomato (Solanum lycopersicum L.) plants under copper stress. Chemosphere, 230, 544–558. https://doi.org/10.1016/j.chemosphere.2019.05.001
[2] Apodaca, S. A., Cota-Ruiz, K., Hernandez-Viezcas, J. A., & Gardea-Torresdey, J. L. (2022). Arbuscular mycorrhizal fungi alleviate phytotoxic effects of copper-based nanoparticles/compounds in spearmint (Mentha spicata). ACS Agricultural Science & Technology, 2(3), 661–670. doi:10.1021/acsagscitech.2c00079
[3] Chen, G., Li, J., Han, H., Du, R., & Wang, X. (2022). Physiological and Molecular Mechanisms of Plant Responses to Copper Stress. International journal of molecular sciences, 23(21), 12950. https://doi.org/10.3390/ijms232112950
[4] Azeez, M. O., Adesanwo, O. O., & Adepetu, J. A. (2015). Effect of Copper (Cu) application on soil available nutrients and uptake. African Journal of Agricultural Research, 10(5), 359-364.

[5] Barragan, Jose Angel et al. “Copper and Antimony Recovery from Electronic Waste by Hydrometallurgical and Electrochemical Techniques.” ACS omega vol. 5,21 12355-12363. 6 May. 2020, doi:10.1021/acsomega.0c01100
[6] Yruela I. (2009). Copper in plants: acquisition, transport and interactions. Functional plant biology: FPB, 36(5), 409–430. https://doi.org/10.1071/FP08288

ESRP: Morphological Characteristics and Cadmium Accumulation in Plants Grown in a Cadmium-rich Environment

Michael Antipov[1], Andrew Bukowski[1], Audrey Cheng[1], Roselyn Deeley[1], Jinan Parves[1], Alice Porfiropoulos[1], Saffron Serber[1], William Wang[1], Nathanael Dille[1], Olga Antipova[2], Wonsuk Cha[2], and David Gosztola[3]

[1]Naperville Central High School, Naperville, IL 60540
[2]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[3]Nanoscience and Technology Division, Argonne National Laboratory, Lemont, IL 60439

Cadmium chloride ($CdCl_2$) is an environmental contaminant found in industrial waste, fertilizers, and fossil fuel emissions [1]. $CdCl_2$ poses risks to human health such as promoting symptoms of nausea, vomiting, and long-term kidney damage [2]. This study investigates the uptake and accumulation of $CdCl_2$ in five plant species with varying cadmium accumulation tendencies – rice, mustard, broccoli, cucumber, and green onion. The plants were cultivated in a controlled agar gel medium infused with increasing $CdCl_2$ concentrations. X-ray fluorescence microscopy (XFM) at the 2-ID-E beamline of the Advanced Photon Source, Raman microscopy, and scanning electron microscopy (SEM) were used to analyze the elemental content and morphology of the plants. The results of this study will contribute to understanding the environmental and agricultural risks of cadmium contamination, with potential applications in food and general contamination safety evaluations.

[1] Centers for Disease Control and Prevention. (2015, March 12). *Cadmium*. Centers for Disease Control and Prevention. https://www.cdc.gov/TSP/PHS/PHS.aspx?phsid=46&toxid=15
[2] Faroon O, Ashizawa A, Wright S, et al. Toxicological Profile for Cadmium. Atlanta (GA): Agency for Toxic Substances and Disease Registry (US); 2012 Sep. 3, HEALTH EFFECTS. Available from: https://www.ncbi.nlm.nih.gov/books/NBK158834/

Quantitative Elemental Masses of Individual Marine Phytoplankton Evaluated with Soft X-ray Spectro-ptychography

Jordan T O'Neal[1,2], Kai Sakurai[1,2,3], Kyota Yoshinaga[1,2], Yu Nakata[1,2], Chiho Funaki[4], Satoshi Matsuyama[5], Yoko Takeo[1,2,3], Takenori Shimamura[1,2,3], Makina Yabashi[2], Haruhiko Ohashi[2,3], Kazutaka Takahashi[4], Mari Shimura[2,6], Taketoshi Kodama[4], and Takashi Kimura[1,2]

[1]Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba, Japan 277-8581
[2]RIKEN SPring-8 Center, Sayo-cho, Sayo-gun, Hyogo, Japan 679-5198
[3]Japan Synchrotron Radiation Research Institute, Sayo-cho, Sayo-gun, Hyogo, Japan 679-5198
[4]Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo City, Tokyo, Japan 113-8654
[5]Research Center for Crystalline Materials Engineering, Graduate School of Engineering, Nagoya University, Nagoya, Japan 464-8601
[6]National Center for Global Health and Medicine, Shinjuku City, Tokyo, Japan 162-8655

Quantifying the masses of light elements C, N, and O within individual marine phytoplankton is critical for understanding complex biological and environmental systems. Traditional methods for measuring light elemental masses require chains of assumptions or aggregating thousands of cells in culture rather than wild specimens. Using a total-reflection Wolter mirror to achromatically focus soft x-rays at SPring-8, we developed a method to measure quantitative masses of light elements in a single, fixed phytoplankton within an hour per element, which could be combined with scanning x-ray fluorescence microscopy (SXFM) to acquire ratios of an array of light and heavy elements in a single cell. This technique involves measuring image stacks by scanning the photon energy across an elemental K-edge with spectro-ptychography (SP). The absolute masses are then extracted from the absorption edge jumps.

We demonstrate the SP methodology for O and Fe in a single centric diatom *Thalassiosira weissflogii* and compare the Fe results to an SXFM measurement of the same cell. The spatial distribution is visualized with edge-subtraction imaging, with comparable resolution for Fe and significantly improved resolution for O due to the larger edge-jump ratio. Further measurements of phytoplankton in the genus *Cylindrotheca* are used to extract the C, N, and O masses in a single cell, demonstrating the ability to rapidly capture an array of light elemental masses.

Advanced Surface Science Approaches to Improve Membrane Protein Crystallization

Hiral P. Patel[1], Arjun Balyan[1], Yin Ma[1], Jierui Sha[1], T. M. Iverson[2], Silvia Russi[3], Aina E. Cohen[3], and Andrew H. Bond[1]

[1]DeNovX, Chicago, IL 60616
[2]Department of Pharmacology, Vanderbilt University, Nashville, TN 37232
[3]Stanford Synchrotron Radiation Lightsource, Menlo Park, CA 94025

With approximately 60% of pharmaceuticals targeting membrane proteins, an understanding of the structure/function relationship is important to various diseases and therapies. Unfortunately, structure determination of membrane proteins remains a challenge owing to their size, hydrophilic/hydrophobic domains, and conformational flexibility. Macromolecular x-ray crystallography remains the benchmark technique for determining protein structures at atomic resolution, and membrane protein crystallization is even more challenging and exceeds the ≈ 85% failure rate in the production of diffraction quality crystals of soluble proteins. DeNovX improves protein crystallization outcomes using a surface science approach while seeking to maintain diffraction quality or to afford seed crystals for growth optimization. Our innovative approaches use bifunctional self-assembled monolayers (bSAMs), surface energy modifications from engineered nucleation features (ENFs), and a hybrid approach using chemically active surface energy modified engineered nucleation features (CENFs). Controlled, replicate, and quantitative crystallization studies have been conducted using these nucleation surfaces with benchmark proteins like insulin, bovine pancreatic trypsin (BPT), and thaumatin. In addition to summarizing the results with soluble proteins, we will present preliminary studies of successful membrane protein crystallization using quinol: fumarate reductase (QFR), flavoprotein subunit A (FrdA), and extracellular signal regulated kinase 2 (ERK2). Replicate studies of the QFR membrane protein show that crystal nucleation and growth behavior can be tuned by using hydrophilic or hydrophobic nucleation substrates. This presentation will include qualitative and quantitative results for crystallization of benchmark and challenge soluble and membrane proteins on a variety of substrates relevant to high throughput screening for traditional and serial crystallography.

ESRP: Comparing Bacterial Gene Expression in Earth and Space Environments

Rahil Bukhari[1], Camden Chiet[1], Kunal Gaind[1], Anthony Herrera[1], Taylor Long[1], Kyna Patel[1], Sophia Rubin[1], Ameya Yammanuru[1], Matthew Bulman[1], and Clark Cucinell[2]

[1]Saint Charles East High School, Saint Charles, IL 60174
[2]Argonne Leadership Computing Facility, Data Science and Learning Division, Argonne National Laboratory, Lemont, IL 60439

As the sector of space exploration has garnered the attention of the world in the past decade, there have been rising concerns about alterations in bacterial behavior in space, specifically concerning microgravity and increased radiation. A large part of bacterial behavior is influenced by gene expression, making our understanding of the changes in gene expression between space and Earth environments crucial to our study. We have done a meta-analysis of the gene expression of three species of bacteria-- *B. subtilis*, *E. coli*, and *S. aureus*-- to identify commonalities between their gene expression in space flight and Earth environments. Using the RNA-seq pipeline in the BV-BRC database, we attempted to identify genes or sequences of genes in the three bacteria that were expressed at altered frequencies. Analysis of the data led us to identify a correlation between the conditions the bacteria were exposed to and their gene expression.

Special thanks to our teacher, Mr. Matthew Bulman, and our research advisor, Mr. Clark Cucinell, from the Argonne Data Science and Learning Division.

[1] (2024). Bv-Brc.org. https://www.bv-brc.org/app/Rnaseq \
[2] Morrison, M.D., Nicholson, W.L. Meta-analysis of data from spaceflight transcriptome experiments does not support the idea of a common bacterial “spaceflight response”. *Sci Rep* 8, 14403 (2018). https://doi.org/10.1038/s41598-018-32818-z
[3] NASA OSDR: Open Science for Life in Space. (2025). Nasa.gov. https://osdr.nasa.gov/bio/repo/data/studies/OSD-95
[4] NASA OSDR: Open Science for Life in Space. (2025). Nasa.gov. https://osdr.nasa.gov/bio/repo/data/studies/OSD-145
[5] NASA OSDR: Open Science for Life in Space. (2025). Nasa.gov. https://osdr.nasa.gov/bio/repo/data/studies/OSD-185

ESRP: Spectroscopic and X-ray Analysis of Cobalamin: Oxidation States and Structural Determination

Tina Vega[1], Ved Sule[1], Ignas Zemaitaitis[1], Jason Augustynski[1], Emma Braathen[1], Madeline Hsieh[1], Maya Ostermann[1], Elyse Smith[1], Joseph Messersmith[1], Sahana Sukumar[2], and Narayanasami Sukumar[3]

[1]York Community High School, Elmhurst, IL 60126
[2]College of Arts and Sciences, Loyola University, Chicago 60660
[3]NE-CAT, Department of Chemistry and Chemical Biology, Cornell University, Building 436E, Argonne National Laboratory, Lemont, IL 60439

Cobalamin (vitamin B12) is a complex biomolecule essential for various biological functions, including enzymatic activity and neurological health. It features a central cobalt ion coordinated by a corrin ring, with its oxidation state and ligand environment playing critical roles in its biochemical functions. In mammals, biologically active forms—adenosylcobalamin (AdoCbl) and methylcobalamin (MeCbl)—serve as cofactors in key enzymatic reactions. Deficiencies in cobalamin metabolism can lead to severe neurological and hematological disorders, highlighting the importance of understanding its structural and electronic properties.

This study investigates the oxidation states of cobalamin using UV-visible spectroscopy and confirms the presence of cobalt through x-ray techniques. Single-crystal x-ray diffraction was attempted to determine its precise molecular structure. UV-visible spectra were collected at Sector 24 (NECAT) at the Advanced Photon Source (APS), while single-crystal cobalamin samples were grown and analyzed at the NECAT 24-ID-E beamline. Additionally, the crystals were sent to NSLS-II for EXAFS scans and anomalous data collection at the Co-edge to further characterize the electronic environment of the cobalt center.

The results of these spectroscopic and x-ray studies will be presented.

CHEMISTRY

A-10

A High Throughput Solvent Sparse Compressive Crystallization Workflow with Detection by Synchrotron Powder X-ray Diffraction and Raman Spectroscopy

Hiral P. Patel[1], Jierui Sha[1], Yin Ma[1], Arjun Balyan[1], Andrey A. Yakovenko[2], Saul Lapidus[2], Tiffany L. Kinnibrugh[2], Douglas Van Campen[3], Apurva Mehta[4], and Andrew H. Bond[1]

[1]DeNovX, Chicago, IL 60616
[2]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[3]Stanford Synchrotron Radiation Lightsource and [4]Linac Coherent Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025

Crystallization is important in the development of pharmaceuticals, of which approximately 90% contain crystalline active pharmaceutical ingredients (APIs) or excipients owing to the cost-effective purity and predictable performance of the crystalline phase. Mechanocrystallization is increasingly used in materials science applications and in the solid form screening of APIs, but the technique is not yet efficient or reproducible in high throughput screening (HTS). To address these shortcomings, our interdisciplinary team developed a workflow that uses compressive comminution, commingling, crystallization, and specimen fixation followed by nondestructive analyses using orthogonal synchrotron powder x-ray diffraction (sPXRD) and Raman techniques on the same specimen without sample transfer losses. The benchmark API cocrystal comprising paracetamol and 2,4-pyridinedicarboxylic acid in a 48 well format with detection by sPXRD gave excellent reproducibility across six continuous variation studies. Additional qualification studies include the mechanochemical preparation and *in-situ* crystallization of a 14 member subset of nicotinamide (a form of vitamin B3 useful in treating niacin deficiency) cocrystals that show 100% agreement in phase preparation and identification by sPXRD relative to published cocrystal phases, along with several previously unreported phases that are being characterized. Exploratory studies include the collection of sPXRD and Raman data on over 4000 specimens during 28 beamtime runs at four beamlines at three synchrotrons. Data collection optimization at the synchrotron beamlines demonstrated that new phases (e.g., cocrystals, hydrates, solvates, and polymorphs) can be reproducibly prepared and identified, with additional high value data including search-match against standard databases for phase identification, semiquantitation of phase fractions without a known structure (critical for screening), and even unit cell indexing. This presentation will include a discussion of the workflow; qualifying studies; the demonstrated benefits that include 2x the analytical data (diffraction + spectroscopic) on the same specimen form factor at a rate 20x faster while requiring 20x less analyte than competing approaches; and our attempts to expand into different sample types for materials science, energy research, and environmental analyses.

Application of Coherent X-ray Reflectivity (CXR) to Image Surface Topography

Anusheela Das[1], Irene Calvo Almazan[2], Ana Suzana[2], and Paul Fenter[2]

[1]Chemical Sciences Division, Argonne National Laboratory, Lemont, IL 60439
[2]Condensed Matter Physics, University of Zaragoza, Zaragoza 50009 Spain

Calcium carbonate is one of the most prevalent salt minerals found in nature, with calcite being its most thermodynamically stable form. The presence of defects in calcite can be influenced by its synthesis process, affecting properties such as mechanical strength, its interactions with heavy metals and its influence on energy storage and catalysis in industrial applications. Therefore, understanding the calcite surface and calcite-water interface is essential, and in this research, we employed coherent x-ray reflectivity to obtain a topographical image of the calcite surface. The growing accessibility of highly coherent beams at next generation synchrotron sources, along with advancements in computational power, has spurred the development of coherent diffraction imaging (CDI) methods. In Bragg coherent diffraction imaging (BCDI), a coherent x-ray beam targets a single particle, and two-dimensional diffraction patterns are captured near the Bragg peak. By stacking these 2D patterns, a three-dimensional Bragg peak is formed, which serves as the basis for reconstructing the phase and electron density of the crystal. In this study, we introduce a coherent x-ray reflectivity (CXR) technique to examine the topography of two-dimensional surfaces, drawing inspiration from the BCDI approach. We show that the three-dimensional diffracted intensity observed around a specific point on the crystal truncation rod (CTR) can be inverted using conventional phase retrieval algorithms to generate a complex density with a distinctive interfacial phase signature.

A-12

Investigating Structural Origin of hTIM4 Cooperative Membrane Binding for Phosphatidylserine (PS) Lipids

Shou-Ting Hsieh[1], Sofiya D. Maltseva[1], Daniel H. Kerr[2], Miah Turke[1], Anna Gaffney[3], Erin J. Adams[4], and Ka Yee C. Lee[1]

[1]Department of Chemistry, University of Chicago, Chicago, IL 60637
[2]NSF's ChemMatCARS, Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637
[3]Program in Biophysical Sciences, University of Chicago, Chicago, IL 60637
[4]Committee on Immunology and Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL 60637

Human transmembrane immunoglobulin and mucin domain protein 4 (hTIM4) is a phosphatidylserine (PS)-binding protein expressed on the membrane surface of many immune cells. hTIM4 utilizes its PS-binding pocket in the IgV domain, mediated by calcium ions, to recognize PS lipids in the target cells, such as apoptotic cells. However, the level of PS exposure in cells varies significantly depending on the cell status. The variation implies that various amount of PS exposure can be a factor to influence binding affinity of hTIM4. In this study, we aim to understand how membrane-binding of hTIM4 responds to the variation of PS exposure and to identify the key molecular contacts of membrane binding. We examined how hTIM4 responds to the variation of PS exposure by using a tryptophan fluorescence assay. The data shows that hTIM4 prefers to bind to vesicles with higher PS mole fractions. Also, we delineated the cooperativity of membrane binding for PS lipid with membrane-binding equation by obtaining the Hill coefficient, $h = 2.18$. To further investigate the key molecular contacts of the cooperativity, we have determined a representative bound structure of hTIM4 by using x-ray reflectivity (XR) combined with molecular dynamics (MD) simulations. Our results shows that the representative orientation from XR fitting is in good agreement with the orientational distribution from all-atom simulations. In addition, the bound structure shows potentially favorable electrostatic interactions between four positively charged residues and negatively charged PS lipids in the vicinity of the binding pocket. Among them, Lys44 and Arg49 frequently contact to PS lipids especially based on the full membrane simulations. Our work shows the cause for cooperative binding nature of hTIM4 in spite of the presence of a single binding pocket and demonstrates the capability of XR combined with MD simulations to identify the membrane-bound structure of a peripheral membrane protein.

ESRP-13

ESRP: Do You Know What's in Your Drink? An Awareness Study on Teen Caffeine Consumption and its Presence in Common Caffeinated Drinks

Alexander Matysik[1], Nathan Leonauskas[1], Andrew Jain[1], Hamid Ali[1], London Shannon-Muscolino[1], Evey McClure[1], Kaitlin Duffy[1], Nicholas Schaller[1], Jenna Eggerding[1], Sarah Wiggins[1], Rhia Nagale[1], Michelle Harbin[1], Debora Meira[2], and H. Christopher Fry[3]

[1]Lyons Township High School, LaGrange, IL 60525
[2]Advanced Photon Source, eBERLight, Argonne National Laboratory, Lemont, IL 60439
[3]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439

Caffeine is a commonly consumed drug around the world, specifically among teenagers, with 73% reporting consuming caffeine through just soda [1]. Social media has promoted caffeine, specifically energy drinks, as being trendy, resulting in the normalization of large quantities of caffeine consumption [2]. Many teenagers are unaware of the negative effects of caffeine, and a large portion do not know the safe daily limit [3]. This study was intended to investigate the popular caffeinated products consumed by adolescents and the actual caffeine content they contain. The significance of this research lies in its potential to raise awareness about the risks associated with caffeine consumption, particularly among teenagers. The research consisted of two main steps. First, a survey was conducted among students at Lyons Township High School to assess their perceptions of caffeine and identify the most commonly consumed caffeinated products. Second, using the data from the survey, UV/Vis spectroscopy was conducted on the most popular caffeinated beverages to identify caffeine content, and then the results were compared with results from High-Performance Liquid Chromatography (HPLC). The survey found that soda and the energy drinks Bubbl'r, Celsius, and Redbull were among the most regularly consumed caffeinated products for Lyons Township High School students. Students often consumed caffeine through sodas, teas, and coffee, with most students consuming at least some amount of caffeine regularly. HPLC results revealed only slight differences between labeled caffeine content and the measured amount of caffeine, with most beverages' caffeine content lining up closely with the advertised caffeine content.

[1] Ebert, M. (2024, May 21). Survey reveals teens' top caffeine sources and parental concern. Contemporary Pediatrics. https://www.contemporarypediatrics.com/view/survey-reveals-teens-top-caffeine-sources-and-parental-concern
[2] Alissa N. A. (2024). The impact of social media on adolescent energy drink consumption. Medicine, 103(19), e38041. https://doi.org/10.1097/MD.0000000000038041
[3] Public Health Agency of Canada. (2018). At-a-glance – Perceptions of caffeinated drinks among youth and young adults in Canada - Canada.ca. Canada.ca. https://www.canada.ca/en/public-health/services/reports-publications/health-promotion-chronic-disease-prevention-canada-research-policy-practice/vol-38-no-5-2018/glance-perceptions-caffeinated-drinks-among-youth-young-adults-canada.html

A-14

Characterization of the Iridium ‘Blue Dimer’ Catalytic Water Oxidation via Optical and X-ray Transient Absorption

Andrew Maurer[1,2], James Wilkes[1], Damith Lekamlage[1], Cunming Liu[2], Jier Huang[1], and Xiaoyi Zhang[2]

[1]Department of Chemistry and Shiller Institute for Integrated Science and Society, Boston College, Boston, MA 02467
[2]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60349

While the importance of oxygen evolution reactions (OER) cannot be understated, our comprehension of ideal system conditions, molecular design, and significant intermediates of champion systems such as the Ir ‘blue dimer’ catalyst is woefully lacking. We have chosen the homogeneous Ir ‘blue dimer’ catalytic system as a suitable candidate for probing photo-driven catalytic OER due to its favorable photochemical properties that allow for careful analysis via optical transient absorption and x-ray transient absorption. Our initial studies have elucidated not only the first oxidation event in the cycle, an oxidation of the Iridium center occurring with a rate of 1.1×10^{5} s^{-1}, but also competitive degradation pathways leading from the unintended reduction of the Iridium catalyst, with a rate of charge transfer on the order of 10^{7} and subsequent degradation occurring through interaction between iridium dimers. Furthermore, the experiments have assisted in the identification of idealized conditions for the catalyst, and photosensitizer, concentration limits and ratios to improve oxidation but restrict reduction events. In addition to kinetic changes through coupling to ns optical transient absorption and simulation of XAS via computational efforts, we are able to model the predicted geometric and coordination changes of the dimer through the oxidation process as well as identify localization of the redox equivalent within the dimer. These efforts additionally set the groundwork for future multipump multiprobe experiments of the same systems.

In-Situ Diffraction and *Ex-Situ* Transmission X-ray Microscopy Studies of Solid-state Upcycling for NMC Cathodes

Matthew L. Nisbet[1], Diana Luong[1], Eva Allen[2], Sohyun Park[1], Tiffany L. Kinnibrugh[3], Joanne E. Stubbs[3], Peter J. Eng[3], John T. Vaughey[1], Tim T. Fister[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439
[2]Applied Materials Division, Argonne National Laboratory, Lemont, IL 60439
[3]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

Direct recycling of lithium-ion battery cathodes offers an alternative source of active cathode materials generated from end-of-life batteries with lower cost and reduced environmental impact compared to virgin battery manufacturing and conventional recycling methods. For batteries using NMC ($LiNi_xMn_yCo_zO_2$) cathodes, upcycling of low-nickel materials such as $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC333) and $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622) can be employed to produce cathode materials with higher capacity due to increased nickel content (i.e. $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$, NMC811). As part of the ReCell Center, we are developing a solid state upcycling method which involves coating the low-nickel NMC material with a nickel-rich precursor phase and a lithium source (e.g. $Ni(OH)_2$ + LiOH) followed by calcination at 900°C to produce a layered NMC811 cathode. In this work, solid-state upcycling of NMC622 via calcination with $Ni(OH)_2$ and LiOH was monitored using *in-situ* synchrotron powder x-ray diffraction and *ex-situ* variable-energy transmission x-ray microscopy measurements. Sequential Rietveld refinements indicate that the calcination proceeds by initially converting $Ni(OH)_2$ to a rocksalt NiO phase followed by lithiation of NiO to form $LiNiO_2$ (LNO), with both NMC and LNO phases present in nearly equal proportions at the calcination endpoint. Variable-energy transmission x-ray microscopy tomograms of upcycled samples reveal that the NMC and LNO domains are intermixed at the primary particle level. Depth-dependent analysis of multi-elemental fitting maps matches the expected NMC811 composition at the secondary particle level and indicates that transition metal diffusion is not limited by the secondary particle size.

This poster has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. All work was funded through the ReCell Center, which is supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy, and the Vehicle Technologies Office. Portions of this work were performed at GeoSoilEnviroCARS (GSECARS) (The University of Chicago, Sector 13), Advanced Photon Source (APS) at Argonne National Laboratory. GSECARS was supported by the National Science Foundation – Earth Sciences (EAR – 1634415). Portions of this research were performed at beamline 18-ID of the National Synchrotron Light Source II, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.

CONDENSED MATTER PHYSICS

A-16

Investigating the Penetration of Indolicidin into Supported Lipid Bilayers Using X-ray Reflectivity and Standing Wave X-ray Fluorescence

Gobind Basnet[1], Jonathan Maloney[1], Jyotsana Lal[1,2], Elizabeth Gaillard[3], and Laurence Lurio[1]

[1]Department of Physics, Northern Illinois University, DeKalb, IL 60115
[2]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439
[3]Department of Chemistry and Biochemistry, Northern Illinois University, DeKalb, IL 60115

To understand the interaction of antimicrobial peptides with biological membranes, we investigated the penetration of indolicidin into supported lipid bilayers (SLBs) using x-ray reflectivity (XRR) and standing wave x-ray fluorescence (SWXF). SLBs were prepared from a 10:1 molar ratio of DMPC and DMPG lipids and incubated with both unlabeled and gold nanoparticle-labeled indolicidin at concentrations of 2, 5, and 10 μM. XRR measurements revealed structural differences between untreated and indolicidin-treated bilayers, while SWXF provided insight into the peptide's depth within the membrane. Results indicate that indolicidin penetration increases with concentration, with bilayers incubated with 10 μM gold-labeled indolicidin exhibiting the deepest insertion, followed by 5 μM and 2 μM. These findings demonstrate how peptide concentration and labeling influence membrane interactions, offering insights into the mechanism of antimicrobial peptide activity.

Generating Entangled X-ray Biphotons

Liam Powers[1] and Stephen Durbin[1]

[1]Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907

The Hong-Ou-Mandel effect is a well-known two-photon interference phenomena in quantum optics [1]. Traditional quantum optics experiments are limited to the optical regime by nature of their sources. We propose a method to extend the Hong-Ou-Mandel effect to the hard x-ray regime with the use of a high-brightness synchrotron source. This would enable the production of entangled biphotons at much higher rates than would currently be possible through traditional parametric down-conversion methods and allow quantum optics techniques to be extended to established x-ray facilities. We outline the construction of a brightness-preserving x-ray interferometer capable of identifying biphoton states along with initial testing and calibration and propose a detection scheme to identify x-ray biphotons produced through Hong-Ou-Mandel interference.

This research was supported by the US Department of Energy under Contract No. DE-SC0023176.

[1] C. K. Hong, Z. Y. Ou, and L. Mandel, "Measurement of subpicosecond time intervals between two photons by interference," Physical Review Letters, vol. 59, no. 18,pp. 2044–2046, Nov. 1987

Kβ X-ray Emission Spectra Analysis Using Bayesian Optimization

Rishabh Ranjan[1], Zichao Di[1], Mark Wolfman[1], Shelly D. Kelly[1], and Chengjun Sun[1]

[1]Argonne National Laboratory, Lemont, IL 60439

The Kβ x-ray emission spectrum (XES) of transition metals is rich with electronic and structural information due to strong exchange interactions with the valence shell of the metal, which is crucial for understanding their spin and oxidation states (Glatzel & Bergmann, 2005). The spectrum is commonly treated using ligand-field multiplet theory (de Groot & Kotani, 2008), a semi-empirical theory that uses parameters to explicitly account for many of the effects present in XES. However, determining the values of these parameters remains a challenge (Huang et al., 2022). We present a new methodology that applies Bayesian optimization to ligand-field theory to determine parameter values. The algorithm is tested on a collection of Mn, Co, and Ni oxides. We demonstrate significantly improved accuracy and provide visualizations of parameter impacts on spectral shape; we are able to find optimal values for up to four parameters and analyze the individual impact of each parameter on both the spectral shape and how certain parameters might be dependent on one another. This advancement will enhance our understanding of transition metal properties, facilitating applications across various scientific fields.

[1] de Groot, F., & Kotani, A. (2008). Core Level Spectroscopy of Solids. Taylor and Francis Group.
[2] Glatzel, P., & Bergmann, U. (2005). High-resolution 1s core hole X-ray spectroscopy in 3d transition metal complexes—electronic and structural information. Coordination Chemistry Reviews, 249(1-2), 65-95.
[3] Huang, I., et al. (2022). The AXEAP2 program for Kβ X-ray emission spectra analysis using artificial intelligence. Journal of Synchrotron Radiation, 29(5), 923-934.

A-19

Investigating CDW and Structural Order in Tetragonal Nematic Candidate $SrAl_4$

Danila Sokratov[1], Prathum Saraf[1], Jared Dans[1], and Johnpierre Paglione[1,2]

[1]Quantum Materials Center, Department of Physics, University of Maryland, College Park, MD 20742
[2]Canadian Institute for Advanced Research, Toronto, Ontario, Canada M5G 1Z8

Electronic nematic order has received significant attention since the discovery of iron pnictides, where nematicity has been shown to lower the superconducting transition of doped $BaFe_2As_2$ through suppressing dynamic fluctuations of competing orders [1]. In a similar but nonmagnetic system, $Ba_{1-x}Sr_xNi_2As_2$, optimally substituted samples displayed a strong nematic response which coincided with a six-fold enhancement of the superconducting temperature [2]. Despite these drastic effects, not many materials display hints of an electronic nematic order, warranting further studies of this phase, especially in the presence of exotic electronic structures.

We explore the transport properties of $SrAl_4$, a member of the $BaAl_4$ structure family which also houses the aforementioned 1-2-2 nematic compounds. The material exhibits a charge-density wave (CDW) order at ~245K and a subtle first-order structural transition at ~90K to a monoclinic structure, both transitions that are absent in the isostructural sister compound $BaAl_4$. Preliminary elastoresistivity measurements carried out on a Razorbill strain cell show that the system is exhibiting signs of an electronic nematic order that may be driving the CDW and structural transitions seen in $SrAl_4$. The sensitivity of the system to a perturbation like uniaxial strain is a sign that other quantum phases, like superconductivity, could be induced.

[1] Malinowski, Paul, Qianni Jiang, Joshua J. Sanchez, Joshua Mutch, Zhaoyu Liu, Preston Went, Jian Liu, Philip J. Ryan, Jong Woo Kim, and Jiun Haw Chu. “Suppression of Superconductivity by Anisotropic Strain near a Nematic Quantum Critical Point.” *Nature Physics* 16, no. 12 (December 1, 2020): 1189–93. https://doi.org/10.1038/s41567-020-0983-9.
[2] Eckberg, Chris, Daniel J. Campbell, Tristin Metz, John Collini, Halyna Hodovanets, Tyler Drye, Peter Zavalij, et al. “Sixfold Enhancement of Superconductivity in a Tunable Electronic Nematic System.” *Nature Physics 2019 16:3* 16, no. 3 (December 23, 2019): 346–50. https://doi.org/10.1038/s41567-019-0736-9.

A-20

Polar and Magnetic Coupling in $PbTiO_3/SrRuO_3$ Heterostructures

Syed Adnan Raza[1], Vladimir Stoica[2], Lane Martin[3], H. G. Lee[4], J. Nordlander[5], M. Hanke[5,]
M. Schmidbauer[6], Venkatraman Gopalan[2], and J. W. Freeland[1]

[1]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[2]Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA 16802
[3]Rice Advanced Materials Institute, Rice University, Houston, TX 77005
[4]Department of Physics, University of California, Berkeley, Berkeley, CA 94720
[5]Paul Drude Institute for Solid State Electronics, Humboldt University of Berlin, 10117 Berlin, Germany
[6]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

Coupling between polar and magnetic order, multiferroics, is a fundamental problem for condensed matter physics. Typically, this coupling occurs at the atomic scale via local interactions between the polar lattice distortion and changes in the magnetic exchange pathways. In this work, we explored the coupling between nanoscale polar super textures and ferromagnetic order of $(PbTiO_3)_{16}/(SrRuO_3)_9/(PbTiO_3)_{16}$ heterostructures on $DyScO_3(110)$ substrates. Using the correct strain state, the $PbTiO_3$ layer forms polar vortices (11nm periodicity) and we have verified the nano scale in-plane strain modulation penetrates into the $SrRuO_3$ layer. We explored the direct charge excitations in Ti and Ru, which are strongly coupled at the interface, via resonant x-ray reflectivity. The results of this study will give further insight into creating nanoscale modulations in magnetic materials.

ENVIRONMENTAL SCIENCE & GEOLOGY

ESRP: Analyzing Air Quality in Aurora Winter 2025, Particulate Concentration and Elemental Composition at Metropolitan Sites

Monserrat Alanis Ramirez[1], Jesus Gonzalez[1], Aylin Mojica[1], Karina Navarro[1], Wyatt Meyer[1], Diane Nead[1], and Antonio Lanzirotti[2]

[1]East Aurora High School, Aurora, IL 60505
[2]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL 60637

This study focused on analyzing a variety of air pollutants throughout the Aurora metro area to compare pollution levels at locations with differing levels of human activity. Air pollution has a recognized potential for significantly impacting human health. Ultrafine particles are correlated to adverse impacts on human health. The composition and density of particles in air that can be inhaled are dependent on local and regional sources of air pollution and weather patterns. In this study we placed low cost, passive air samplers, modified after designs published by Castillo et al. [1] in the Aurora, IL area with the goal of assessing if regional differences in air quality are identifiable using such low-cost air samples. We evaluated our samples using microscopy (SEM) to determine the concentration of pollutants and some elemental analysis to determine what sort of materials were in the air samples. Samples were collected at a local forest preserve (Oakhurst Forest Preserve), the community high school (East Aurora High School), near a vehicular bridge over multiple train tracks, and a more commercial/industrial location (intersection of Indian Trail and Orchid roads) in the city. Elemental analysis identified sodium (Na) and chlorine (Cl) at all locations except at the Oakhurst Forest Preserve. Other chemicals found were silicon, calcium, chlorine, sulfur. These findings highlight the need for further investigation into air pollution sources and mitigation strategies in the Aurora, IL metro area.

[1] Castillo, M. D., Wagner, J., Casuccio, G. S., West, R. R., Freedman, F. R., Eisl, H. M., ... & Kinney, P. L. (2019). Field testing a low-cost passive aerosol sampler for long-term measurement of ambient PM2. 5 concentrations and particle composition. *Atmospheric Environment*, *216*, 116905.

ESRP: Exploring Environmental Contamination from Resource Processing in Plant Structures in the Joliet Area

Horacio Almazan[1], Amber Beach[1], Fernando Chavez Guzman[1], Noemi Herrera-Rodriguez[1], Ozziel Lara[1], Adan Martinez[1], Elizabeth Meza[1], Juvelda Missamou Batotana[1], Josephine Nudi[1], Breanna Ocupe[1], Mariana Reyes[1], Jimmy Sanchez[1], Alexa Villalpando,[1] Constance Pfeiffer[2], Rachel Koritala[2], and Lauren Kline[1]

[1]Science Department, Joliet Central High School, Joliet, IL 60432
[2]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439

Joliet, the largest city in Will County, is known for the significant production of energy and steel [1]. Producing these resources can lead to high levels of contamination, which could affect the day-to-day lives of Joliet residents [2]. Samples were collected at the site of study (a power generating station) and various locations around the area. A Scanning Electron Microscope (SEM) was used to obtain information about the elemental makeup of each sample and collect data on plant structure and composition, looking for anomalies in various plant structures or elemental composition. While the experiment is still underway, examining SEM images of the plants and their composition for any signs of contamination gives insight into the impact of generating stations and other production industries. The results of this study can invoke future researchers to investigate contamination in or around the area.

[1] Reconnect with Nature. (n.d.). *Steeling Joliet: Past iron works at historic site*. Reconnect with Nature. https://www.reconnectwithnature.org/news-events/big-features/steeling-joliet-past-iron-works-historic-site/
[2] U.S. Environmental Protection Agency. (n.d.). *Human health and environmental impacts of the electric power sector*. U.S. Environmental Protection Agency. https://www.epa.gov/power-sector/human-health-environmental-impacts-electric-power-sector

ESRP: Root Uptake of Iron in Common Plants and Vegetables

Lauren Ascolani[1], Tori Averill[1], Max Bruzga[1], Miriam Fahmy[1], Alexander Lazarowicz[1], Jovana Maksimovich[1], Olivia Parent[1], Krisha Patel[1], Om Patel[1], Emily Perry[1], Huai-Yu Peng[1], Anika Reddy[1], Alexandra Reyna[1], Ceren Sarac[1], Kevin Schmitt[1], Lauren Tracy[1], Erin Horan[1], Wonsuk Cha[2], David Gosztola[3], Elena Rozhkova[3], and Olga Antipova[2]

[1]Lemont High School, Lemont, IL 60439
[2]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[3]Nanoscience and Technology Division, Argonne National Laboratory, Lemont, IL 60439

In plants, iron is a vital micronutrient due to its use in various physiological and biochemical processes. Iron is naturally found in soil and plants, but the additional uptake of iron in plants comes from secondary oxides that are derived from pollution. This iron is highly poisonous to plants when seen in abundant quantities. Excess iron intake leads to stunted roots and leaf discoloration. Iron toxicity may also affect the uptake and distribution of other vital elements within the plant tissues, stomata, or chloroplasts. Recent concerns cover iron-rich pollution that is being increasingly emitted from industry and traffic-related sources. This research shows how levels of iron interfere with the plants' biological systems. The common plants and vegetables studied are commonly grown in areas that are rich in iron pollution. Iron in the human body is a necessity, but, if iron is excessively consumed, it can lead to health issues. Through Lemont High School's Exemplary Student Research Program (2018-2025), students have had the ability to work closely with Dr. Olga Antipova (Argonne National Laboratory) to examine the relationship between the contamination of common vegetables while in the seedling stage of growth and their root uptake of toxic heavy metals with a focus on iron. During the 2023-2024 ESRP experiment, the research group used the Raman microscopy to evaluate chlorophyll levels and SEM EDX that revealed ultrafine structures of plant tissues but was not as sensitive and showed little to no uptake of iron. For 2024-2025, the samples were grown and retested using the Raman microscopy and SEM EDX along with the use of more sensitive X-ray Fluorescence Microscopy (XFM) at the 2-ID-E beamline of the Advanced Photon Source, which revealed iron and micronutrients distribution in response to iron stress. We examined the growth and stress signs of carrots, lettuce, and tomatoes in an iron-rich environment with iron citrate or iron oxide particles and evaluated the difference in iron in roots and leaves to determine the long-term impact of iron pollution on the edible plants.

HIGH PRESSURE

A-24	**Chariton, Stella**
A-25	**Giaimo, Michael**
A-26	**Prakapenka, Vitali**
A-27	**Ryu, Young Jay**
A-28	**Yakovlev, Maksim**
A-29	**Zhang, Dongzhou**

The 13-ID-D High-pressure Beamline Upgrade: New Opportunities for Studying Materials at Extreme

Stella Chariton[1], Vitali Prakapenka[1], Dongzhou Zhang[1], Mark Rivers[1], Peter Eng[1], Mike Proskey[1], and Christofanis Skordas[1]

[1]The University of Chicago, Center for Advanced Radiation Sources, Lemont, IL 60439

The 13-ID-D high-pressure x-ray diffraction beamline at GSECARS (APS, USA) has proudly served hundreds of diamond anvil cells (DAC) users worldwide in the past 25 years. The APS-U has introduced a new era of significant technical advances in hardware, software, and emerging techniques at 13-ID-D. The user community will be greeted with compelling features, such as hundreds of times more brightness on a 300 nm x-ray focused beam, new high precision stages for smooth sample motion, a vibration-free granite base table, an Eiger2 9M CdTe detector with high spatial resolution, a revised double-sided laser heating system with updated optical layout, an optimized high-resolution on-line Raman spectroscopy system, a supercontinuum laser for reflectivity/absorption measurements at high temperatures in the laser-heated DAC, as well as updated user-friendly software, operation protocols, and supporting labs. These cutting-edge developments stimulate research at multi-Mbar pressures, where novel compounds such as superconductors or ultra-incompressible materials can be synthesized, and super-Earth planetary interiors can be studied. Analytical methods such as single-crystal x-ray diffraction on complex multiphase/multigrain samples, fine 2D x-ray diffraction mapping with sub-micron precision, high-pressure x-ray diffraction at high or cryogenic temperatures, and dynamic compression in the laser-heated DAC are only some of the many new capabilities that 13-ID-D highlights.

Rock-fluid Interaction in Ice and Gas Giant Planets

Michael Giaimo[1], Suzanne Autrey[1], Oliver Tschauner[2], Stella Chariton[3 4], and
Vitali Prakapenka[3,4]

[1]Department of Earth, Atmosphere and Environment, Northern Illinois University, DeKalb, IL 60115
[2]Department of Geoscience, University of Nevada, Las Vegas, NV 92093
[3]GeoSoilEnviro Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60439
[4]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

Mg and Fe-bearing silicates are the most abundant rock-forming minerals in primitive meteorites and in the rocky fractions of comets [1,3]. Thus, they are expected to form the major fraction of rocky material in the interior of Uranus, Neptune, and Saturn and perhaps giant exoplanets. There are indications that rocky material reacts with the low-Z material in these planets [2]. We explore high-pressure-high temperature reactions of olivine with low Z-fluids in the range of 10s of GPa and several thousands of K by combining shock-induced deflagration and shock reverberation. Samples are examined by synchrotron micro-diffraction at the APS, beamline 13-ID-D, by Raman spectroscopy at GSECARS, and FE-EPMA.

[1] Mason, B., 1963, Olivine composition in chondrites: Geochimica et Cosmochimica Acta, v. 27, p. 1011–1023, doi:10.1016/0016-7037(63)90062-0.
[2] Militzer, B., Wahl, S., and Hubbard, W.B., 2019, Models of Saturn’s Interior Constructed with an Accelerated Concentric Maclaurin Spheroid Method: The Astrophysical Journal, v. 879, p. 78, doi:10.3847/1538-4357/ab23f0.
[3] Zolensky, M., Engrand, C., Nakamura, T., and Ebel, D., 2024, Composition and Mineralogy of Nuclei Material of Short Period Comets Revealed by Recent Spacecraft Missions: Space Science Reviews, v. 220, p. 79, doi:10.1007/s11214-024-01111-z.

A-26

Diamond Anvil Cell Program at GSECARS after APS-U

Vitali B. Prakapenka[1], Stella Chariton[1], Young Jay Ryu[1], and Dongzhou Zhang[1]

[1]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL 60637

The Advanced Photon Source is opening again for research after a complex upgrade. The original electron storage ring was replaced with a new multi-bend achromat lattice to provide extremely enhanced coherent flux and increased hard x-ray brightness by a hundred times. To take full advantage of these improved capabilities we have started the process of comprehensive technical improvements and developments of multi-probe techniques across a suite of beamline stations at GSECARS.

The laser-heated DAC technique combined with high energy tightly focused x-ray beam and fast detectors for spectroscopic measurements is the workhorse method for exploration of deep Earth mineral physics and chemistry. To provide new constraints on models for planetary evolution and origin, essential properties (melting, structure, phase relation, chemical reactions and kinetics, transport, elastic, electronic and optical properties) of a wide range of minerals must be studied *in situ* at extreme conditions of pressure and temperature. However, existing data sets are often inconsistent or poorly constrained to provide unique answers. This underscores the need for unique beamline capabilities: high-energy high-flux sub-micron x-ray beam to probe ultra-small samples (micron-sized) in megabar pressure range, high resolution large area fast x-ray and optical detectors for time-domain experiments, sample emissivity and absorption measurements to improve radiative temperature metrology, etc. To accomplish that we will install a vibration-free granite-table system at 13-ID-D station coupled with pre-shaped sub-micron x-ray focusing system (300 nm) and high precision sample positioners including an air-bearing rotary stage, long focal length optical spectrometer, and a new Eiger2 CdTe 9M X-ray detector. We plan to upgrade the x-ray and laser optics (Raman, Brillouin, fluorescence, absorption) at 13-ID-D, 13-BM-C, and 13-BM-D stations to accommodate higher x-ray energies in a tighter focused beam, which grants a significant boost in the reciprocal space explored at high temperatures with increased spatial resolution.

Recent results and details of future developments of the cutting-edge synchrotron and optical techniques for comprehensive characterization of materials *in situ* at extreme conditions will be discussed.

A-27

Recent and Future Development in Extreme Conditions Research at GSECARS 13-BM-D

Young-Jay Ryu[1], Vitali Prakapenka[1], Stella Chariton[1], Dongzhou Zhang[1], and
Stanislav Sinogeikin[2]

[1]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL 60637
[2]DacTools, LLC, Downers Grove, IL 60515

The scientific goal of the diamond anvil cell program at GSECARS (GeoSoilEnviro Center for Radiation Sources) 13-BM-D is to investigate materials across the entire pressure and temperature conditions that exist on terrestrial planets. This research relies on a variety of high-pressure measurement techniques that operate under extreme conditions. Our primary goal is to significantly expand the range of pressure and temperature that can be explored in high-pressure experiments. At the same time, we aim to improve the accuracy of the experimental data collected by developing techniques, ensuring that our findings are reliable and valuable for advancing scientific knowledge.

During the Advanced Photon Source Upgrade (APS-U), we newly developed a resistive heating device for diamond anvil cells, along with their enclosures. These devices are highly versatile and sophisticated, making them suitable for a wide range of applications in geoscience research, including but not limited to condensed matter physics, material science, and chemistry. The newly designed diamond anvil cells and their enclosures create a stable and uniform thermal environment. This capability is crucial because it allows researchers to simultaneously study synchrotron x-ray, Brillouin spectroscopy, and Raman spectroscopy at high pressure and temperature (≤1600 K). This combination allows the geoscience community to study behaviors of various materials, including minerals and synthetic compounds, under conditions that mimic those found deep within the Earth or other rocky planets. In addition, they may offer a unique and invaluable opportunity to explore the fundamental properties and behavior of materials in extreme environments, which can lead to breakthroughs in our understanding of geological processes and the formation of planetary bodies. We will discuss more details in the presentation.

Reconstruction Correction for Low-signal, Artifact-prone High Temperature and Pressure Microtomography Datasets in Earth Science

Maksim A. Yakovlev[1], Yanbin Wang[1], Timothy Officer[1], Tony Yu[1], Man Xu[1], Geeth Manthilake[2], Tahar Hammouda[2], and Mark Rivers[1]

[1]Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL 60637
[2]Laboratoire Magmas et Volcans, Université Clermont-Auvergne, 63170 Aubière, France

The *in-situ* study of geological processes occurring in the upper mantle is challenging not just due to the necessary replication of the associated high pressure and temperature conditions but also due to the opaque nature of the samples and the containment surrounding them. Imaging using synchrotron micro computed tomography (micro-CT) of such samples enables the rapid acquisition of large, highly detailed 3-dimensional (3D) datasets, but the replication of high pressure and temperature conditions via a Paris-Edinburgh (PE) press and heating elements leads to artifacts in the final reconstructed images. These errors are mostly due to three factors – a low signal-to-noise ratio (SNR) associated with x-ray attenuation throughout the PE press and uncontrolled vertical and horizontal motions associated with the mechanical difficulty of keeping uniform movement of a one-ton press at high pressures. These inaccuracies in motion are not reproducible between individual scans under identical pressure conditions and obfuscate the resulting image data with large streaks which blur out objects of interest. Here, we present an image processing pipeline that improves the quality of the raw acquired images and enables qualitative and quantitative segmentation-based analysis of potential gaseous bubble formations at varying temperatures and pressures for a study of magma formation. Motion correction starts in the sinogram domain by tracking individual, highly attenuating features as they translate across sinograms (for vertical motion) and take an inaccurate sinusoidal path (for horizontal motion). The low SNR of the sinograms necessitates signal boosting in specific scans, accomplished by a combination of FFT image cropping and median filtering. Once detected, the path of these objects is rectified by shearing the dataset, aligning the same feature to a single vertical slice, and forcing the semi-sinusoidal track to a sine wave whose period corresponds to the number of projections taken over a single, 180-degree scan. Reconstruction of these corrected datasets allows the visualization and segmentation of otherwise undetectable features, functionally boosting the resolution of the high pressure/temperature micro-CT machine at GSECARS. Our future plans for implementing and improving this method center on the inclusion of highly attenuating markers within the field of view for easier tracking of features.

A-29

High Pressure Research at GSECARS 13-BM-C after the APS Upgrade

Dongzhou Zhang[1]

[1]GeoSoilEnviroCARS, University of Chicago, Lemont, IL 60439

The GSECARS 13-BM-C beamline at the Advanced Photon Source has been providing crystallographic research capabilities to the high-pressure community since 2015. This beamline utilizes focused x-rays at 29 keV and a unique 6-circle heavy duty diffractometer to carry out advanced crystallographic research. The instrument is optimized for a variety of advanced crystallography experiments including interface studies, powder and single crystal structure determination, equation of state studies, optical spectroscopy, and atomic dynamics research. Currently we support high-pressure and variable-temperature experiments using diamond anvil cells, resistive-/laser-heating and cryostats. We have achieved P-T conditions of 100 GPa and 150-3000 K. Results of multiple recent experiments, including powder and single crystal diffraction over a range of P-T conditions, equations of state and atomic dynamics will be presented to demonstrate the experimental capabilities. These new capabilities are available to all researchers interested in studying deep earth materials through the APS General User Program.

INSTRUMENTATION

A-76	**Alatas, Ahmet**
A-77	**Arzoumanidis, Alex**
A-78	**Beavers, Christine**
A-79	**Carpenter, Andrew**
A-80	**Fram, Andrew**
A-81	**Gironda, Anthony**
A-82	**Gray, Christopher**
A-83	**Han, Josh**
A-84	**Jiang, Jinxing**
C-85	**Riccio, Mark**
A-87	**Tian, Jiajun**
A-89	**Rivers, Mark**

High-energy-resolution Inelastic X-ray Scattering Spectrometer at the Advanced Photon Source (30-ID)

A. Alatas[1], A. H. Said[1], and M. Y. Hu[1]

[1]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

Inelastic x-ray scattering is a powerful and versatile technique for studying lattice dynamics in materials of scientific and technological importance. An overview of the momentum-resolved high-energy-resolution inelastic x-ray spectrometer (HERIX), 1.5 meV energy resolution, at beamline 30-ID of the Advanced Photon Source (APS) will be presented, including the recent results from the upgraded APS storage ring.

In addition to the HERIX spectrometer at sector 30, the beamline offers Nuclear resonant scattering (NRS) capabilities. NRS is used to study atomic dynamics and electronic properties of archetype and functional materials to determine the partial density of states. 30-ID NRS instrument focuses on tin-containing samples using isotope Sn-119.

Both spectrometers are fully commissioned and open to general user program at the APS.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility at Argonne National Laboratory and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Radiograph Post-process Runout Correction for *In-situ* Micro-CT Mechanical Tests

Alex Arzoumanidis[1], Zach Thompson[1], Brian K. Bay[2]

[1]Psylotech, Inc. Evanston, IL 60201
[2]Department of Mechanical, Industrial and Manufacturing Engineering, Oregon State University, Corvallis, OR 97331

A process is presented that uses imaging metrology to potentially achieve sub-micron Digital Volume Correlation displacement field resolution. An x-ray tomography compatible twin post universal test machine has been developed, offering a number of advantages. For example, compared to tubular frame alternatives, no x-rays are blocked, and sample access is simplified. Additionally, the source can be placed near the sample, maximizing resolution for conical beam tomography. However, rotating the load train introduces two rotation axes, complicating *in-situ* testing. The top and bottom actuators which must be aligned to each other and also to the scanner's rotation axis. Moreover, two sets of bearings introduce radial and axial runout, causing aberrations in 3D reconstructions. Micron-scale mechanical alignment solutions are presented, but the ultimate goal is sub-voxel Digital Volume Correlation metrology on sub-micron resolution x-ray tomography.

Spherical fiducial markers are bonded to the top and bottom of the sample’s gauge section with a low modulus adhesive. The markers are tracked in all the radiographs of the tomography scan, presenting a sub-voxel resolution runout and alignment measurement. The marker locations are curve fit in space to find the rotation axis of both the top and bottom actuator. Each radiograph is then shifted and distorted into proper alignment and corrected for runout. Axis alignment and tilt errors have been successfully corrected. Pitch errors remain a work in progress.

56,000 fps Hybrid Pixel Array X-ray Detector: Aiming for Time Resolved and Imaging Experiments

Y. Nakaye[1], C. Beavers[1], T. Sakumura[2], Y. Sakuma[2], and S. Mikusu[2]

[1]Rigaku Americas Corporation, The Woodlands, TX 77381
[2]Rigaku Corporation, Akishima-shi, Tokyo 196-8666, Japan

It has been more than ten years since HPAD (Hybrid Pixel Array Detectors) have been widely utilized as x-ray diffraction and imaging detectors. Thanks to their single photon counting capability, HPADs give images without background noise and with a wide dynamic range. Due to limitations of the fabrication process, most HPADs are made with a monolithic sensor and tiled readout ICs. In a conventional HPAD, there were so-called “inter-chip pixels” on the edges of the readout ICs. These inter-chip pixels are 1.5 times wider and/or taller than non-inter-chip pixels. This means we are losing position information for photons impinging on those pixels.

We have successfully dealt with this inter-chip pixel problem by using a re-distribution layer on the Silicon sensor. So, in this detector, non-uniformity in a single sensor module is eliminated.

This new detector is designed based on UFXC32k IC [1] and its high energy resolution variant LNPX32k IC for soft x-ray application detector, both designed by AGH University of Science and Technology and named the XSPA [2] detector series. XSPA detectors employ modulated design with each monolithic sensor module consists of 16 UHXC chips tiled and 1024 x 512 76 um sq. pixels. The absence of inter-chip pixels between ROICs leads to improved image quality.

The XSPA detector series is aiming not only for x-ray imaging but also for time-resolved x-ray measurements. Dealing with “inter-chip pixels” is our main feature for imaging, and for time-resolved measurements we understand that frame rate is as important as the size of the pixels and the area of the detector. Thanks to UFXC32k IC’s high count-rate and fast operation capability, combined with our high data throughput backend circuits, XSPA-500k is capable of up to 56,000 fps with full-frame readout and 100,000 fps with 100 lines ROI in the centre of the modules with continuous exposure (zero-deadtime mode operation with 2-bit counter/pixel.) If the non-continuous exposure (burst-mode operation [3]) is allowed, it can achieve over 970,000 fps with approximately 2% duty ratio. By using its variant LNPX32k IC, we can operate our detector with as low as 400 eV x-ray and working on finding the best parameter set that work with much lower energy x-ray.

[1] P. Grybos *et al.*, *IEEE Trans. Nucl. Sci.* 63 no. 2, 1155-1161 (2016).
[2] Y. Nakaye *et al.*, *J. Synchrotron Rad.* 28, 439-447 (2021).
[3] Q. Zhang *et al., J. Synchrotron Rad.* 25, 1408-1416 (2018).

Speeding Up EUV and X-ray Detection for a "Brighter" Future

Andrew P. Carpenter[1]

[1]Oxford Instruments Andor, Belfast, Northern Ireland BT12 7AL, United Kingdom

X-ray imaging and spectroscopy continues to yield innumerable contributions in material science, life science, geological science, and beyond. Looking towards the future, high energy sources (i.e., synchrotrons, XFELs, etc.) possess a higher brilliance, higher repetition rates, and higher time resolution. These advances are paving the way for the development of new experimental methodologies and opening the door for the acquisition of large amounts of data. Concurrent with the development of these new high energy sources is the need for advances in x-ray camera technologies that can facilitate the high-throughput generation of data and be incorporated in complex experimental geometries. Importantly, it is critical these camera technologies do not compromise on sensitivity and accuracy of detection while exploiting the higher frame rates of these next generation sources to benefit time-consuming applications (i.e., tomography).

We present several detection solutions for the new high energy sources of the future that are brighter and faster than previous generations. These detection solutions, based on sCMOS camera technology, include direct detection methods for the EUV – soft x-ray regimes and indirect detection methods extending sensitivity into the hard x-ray energies. Looking towards higher brilliance sources and high-throughput methodologies we highlight full frame acquisition rates an order of magnitude, or more, faster than comparable CCD technology while maintaining a high QE and lower noise floor. Further discussion around these cameras is framed in the context of how they can contribute to current experimental methodologies, quickly generate large amounts of data, and how they can facilitate the continual evolution in x-ray methodologies into the future.

5D X-ray Image Processing: Overcoming Big Data Challenges in Synchrotron Science

Andrew Fram[1], Martin Huth[1], Björn Eckert[1], Petra Majewski[1], Lothar Strüder[2], and
Heike Soltau[1]

[1]PNDetector GmbH, Otto-Hahn-Ring6, 81739, München, Germany
[2]PNSensor GmbH, Otto-Hahn-Ring6, 81739, München, Germany

Modern x-ray imaging techniques generate vast amounts of data, presenting significant challenges in data acquisition, processing, and analysis. The Color X-ray Camera (CXC) utilizes a backside-illuminated pnCCD detector capable of counting over 1,000,000 x-ray events per second with an energy resolution of 150 eV at Mn-Kα. This technology enables simultaneous x-ray diffraction and fluorescence imaging, but at the cost of overwhelming data rates—exceeding 140 MB/s and reaching terabytes of raw data in extended experiments. Efficient data processing strategies are therefore essential for extracting meaningful scientific insights.

This work presents a robust pipeline for processing 5D x-ray datasets, where the five dimensions correspond to Sample X, Sample Y, Camera X, Camera Y, and Energy. To mitigate data overload, raw images are first transformed into event lists and then structured into multidimensional data cubes, reducing the data rate to under 150 MB per hour. To improve data quality, we implement advanced noise reduction and data imputation techniques. A biorthogonal wavelet denoising approach significantly reduces Poisson noise while preserving spatial resolution, and missing or incomplete data are reconstructed using singular value decomposition (SVD)-based imputation via the softImpute algorithm.

Separating fluorescence and diffraction signals is another critical challenge. We apply Bragg’s law fitting at the pixel level, filtering out overlapping diffraction signals to produce clean fluorescence-diffraction datasets. This automated approach allows rapid and accurate identification of crystallographic and elemental composition data from high-throughput x-ray imaging experiments. Additionally, event classification and centroid calculations are optimized through parallelized processing, accelerating analysis while maintaining precision.

The proposed methodology is particularly suited for synchrotron-based mapping and imaging experiments where rapid acquisition rates and complex datasets demand efficient and scalable processing solutions. By integrating Python-based tools (PyWavelets, fancyImpute, and ndimage) with parallel computing techniques, we demonstrate a significant improvement in data handling efficiency without compromising scientific accuracy.

This study provides a scalable framework for handling high-dimensional x-ray datasets and offers a pathway for future advancements in synchrotron imaging, materials characterization, and big data-driven spectroscopy. Our approach not only enhances real-time data processing capabilities but also paves the way for broader applications in high-throughput x-ray imaging environments.

New Approaches to X-ray Raman Scattering and HERFD Spectrometers at APS 25-ID

Anthony Gironda[1], Yanna Chen[2], Mark Wolfman[2], Charles Cardot[1], Chengjun Sun[2], Gerald Seidler[1], and Shelly Kelly[2]

[1]University of Washington, Seattle, WA 98195
[2]Argonne National Laboratory, Lemont, IL 60439

The most common technical approaches to x-ray Raman scattering (XRS) and high-energy resolution fluorescence detection (HERFD) make use of spherically bent crystal analyzers (SBCA). The recent work of Gironda, et al., 2024, proposes that asymmetric implementations of the Rowland circle for SBCA can both increase their flexibility of use and also suppress Johann spectral broadening. The latter detail especially supports the use of the latest generation of 0.5-m radius of curvature SBCA, thus increasing detection solid angle while also decreasing spectrometer complexity and cost.

We report here progress at 25-ID on asymmetric implementations of SBCA for both XRS and HERFD. The first highlight is commissioning results for XRS that guide us to an improved spectrometer design for XRS that achieves the benefits of asymmetric operation while retaining imaging capability to reject scatter from sample container windows. This requires a new spectrometer configuration that uses the sagittal focal plane behind the Rowland circle instead of the traditional meridional plane at the Rowland circle. These results are leading us to a compact, modular design for a future APS XRS instrument at 25-ID. The second highlight is continued work on HERFD where the energy-range flexibility of asymmetric SBCA spectrometers has been harnessed for a 1-SBCA prototype instrument that aims to make HERFD operationally simpler for both beamline scientists and users. The long-term goal is that a user could, for example, choose any emission line for a 3-*d* transition metal and the spectrometer would immediately adapt to that choice without beamline scientist intervention.

This work is supported by funding from the U.S. Department of Energy in the Nuclear Energy University Program under Contract No. DE-NE0009158. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility, operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. We thank each of Mali Balasubramanian and Pieter Glatzel for useful discussions, Shelly Kelly and Chengjun Sun for beamline assistance, and Abdullah Ceylan and Abdul Rumaiz for providing the thin film sample studied by HERFD XAS.

“Vacuum Measurement Technology Does Not Have to be Fast!” Not at All! How the View of Transient Vacuum Processes is Made Possible

Christopher Gray[1], Kristian Kirsch[1], Sebastian Röhrig[1], Andreas Trützschler[1], and
Klaus Bergner[1]

[1]VACOM Vakuum Komponenten & Messtechnik GmbH, 07751 Großlöbichau, Germany

In terms of the increasing complexity of industrial processes in vacuum, the quality of the vacuum itself gains more and more impact. To deal with this challenge one crucial aspect is the necessity of monitoring and capturing the pressure and the residual gas composition during the process. Only this way it is possible to react *in situ* during the process to minimize production errors and avoid failures or major damage. However, the measurement speed of hot cathodes or QMS is not sufficient in this process.

One answer to this challenge is our novel ion source NOVION™, which transforms the well-known technology of time-of-flight spectroscopy into an industrially available application.

In this talk, we present the new fundamental physical principles of the novel ion source. Furthermore, we discuss the advantages and limits in the different operation conditions. On the one hand we demonstrate the capability of precise total pressure measurements over a wide pressure range. On the other hand, we show the available possibilities to use the novel ion source in partial pressure measurement mode. Besides the simple use case as He-leak detector to identify air leaks of the vacuum system, the novel ion source is able to quickly access the complete composition of the process gas over the whole process line. For explanation we show different use cases at different pressure levels and discuss physical and technical limits of the novel ion source.

Enabling Multiscale X-ray Imaging of Complex Matrices through Xenon Plasma Focused Ion Beam Milling

Josh Han[1], Tugba Isik[1], Xiaozhi Zhang[1], Benjamin F. Davis[1], Yuzi Liu[2], Ajith Pattammattel[3], Olga Antipova[1], Fabricio S. Marin[1], Kenneth Kemner[4], and Si Chen[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Nanoscience and Technology Division, Argonne National Laboratory, Lemont, IL 60439
[3]National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY 11973
[4]Biosciences Division, Argonne National Laboratory, Lemont, IL 60439

Focused Ion Beam (FIB) milling is an emerging technique for preparing samples for nano-scale x-ray imaging methods, such as x-ray fluorescence microscopy (XFM) and tomography. Traditionally, gallium-based FIB systems, while effective, often introduce metal contamination and are limited by milling rates [1]. The advent of xenon (Xe) plasma FIB (PFIB) technology addresses these limitations by offering substantially higher milling speeds and minimizing sample contamination due to the inert nature of Xe [1,2]. This advancement is particularly critical for large-volume and delicate specimens, enabling more efficient and precise cross-sectioning with minimal structural disruption [2]. In this presentation, we will report on the upgrade of a FIB system with a Xe source and its performance characterization, including the beam profile, Xe deposition, and milling precision.

Additionally, we will present our initial efforts to creating soil samples for subsequent XFM tomography. The application of Xe PFIB is transformative for analyzing complex, heterogeneous systems such as soil samples. Soil aggregates comprise intricate networks of minerals, organic matter, and microbial communities, all closely linked to ecological functions. Conventional preparation techniques such as chemical etching or mechanical sectioning often fail to preserve the native architecture of these samples, hindering accurate analysis. Xe PFIB enables precise milling of millimeter-sized soil samples, while maintaining their native structure. In conjunction with x-ray analysis, we aim to bridge the spatial gap between bulk aggregates and individual microbes, facilitating multiscale analysis of soil aggregates.

[1] Mayr, S., et al. (2021). Xenon Plasma Focused Ion Beam Milling for Obtaining Soft X-ray Transparent Samples. Crystals, 11(5), 546. https://doi.org/10.3390/cryst11050546
[2] Vitale, S. M. & Sugar, J. D. (2022). Using Xe Plasma FIB for High-Quality TEM Sample Preparation. Microscopy and Microanalysis, 28(3), 634–643. https://doi.org/10.1017/S1431927622000344

Selecting and Slicing Ultrashort Synchrotron X-ray Pulses with Picosecond Resolution

Jinxing Jiang[1,4,5], Jian Zhou[1,2,6], Donald A. Walko[1], Daniel Lopez[3], David A. Czaplewski[2], and Jin Wang[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[3]Materials Research Institute, Penn State University, University Park, PA 16802
[4]Department of Physics, University of Illinois at Chicago, Chicago, IL 60607
[5]ChemMatCARS, Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637
[6]Department of Mechanical Engineering, Binghamton University, Binghamton, NY 13902

The fourth-generation synchrotron sources deliver highly brilliant x-rays and revolutionize experiments that depend on coherent x-ray photons. Coherence is achieved in part by extending electron bunch lengths, which results in longer x-ray pulses and consequently limits the time resolution of ultrafast experiments determined by the pulse length. To tackle this challenge, we present a torsional microelectromechanical resonator-based x-ray optics system capable of selecting and slicing ultrafast x-ray pulses with picosecond precision.

Operating at the $2P_0$ resonance mode (P_0 = 271 kHz, the storage ring frequency), the resonator device achieves an angular velocity exceeding 10^7 degree/s while maintaining stability below material breakdown limits. By synchronizing a torsional microelectromechanical resonator with the Advanced Photon Source storage ring, we achieve x-ray pulse manipulation from nanoseconds down to 40 ps [1] by leveraging the narrow Bragg peak of the single-crystalline resonator. The inherent Bragg angle amplification effect enables ultrahigh phase and picosecond time resolution. Even with the extreme phase sensitivity induced by minimal temperature variations, the implemented real-time feedback algorithm successfully stabilizes pulse manipulation to ensure high time resolution with minimum timing jitters.

These advancements position microelectromechanical resonator-based ultrafast x-ray optics as a powerful tool for selecting and slicing synchrotron x-ray pulses, enabling high-resolution dynamic studies beyond current synchrotron temporal limits.

This work is supported by a grant from the DOE/SC/SUF's Accelerator and Detector Research Program. It used the APS (7-ID) and CNM at ANL, DOE SC Scientific User Facilities operated by ANL under Contract No. DE-AC02-06CH11357. We also thank D. Jin of CNM for his technical assistance and discussion.

[1] J. Zhou, J. Jiang, et al., "On-chip picosecond synchrotron pulse shaper," *arXiv preprint arXiv:2211.03567* (2022).

C-85

Unveiling Dynamic Materials Behavior at the Atomic Scale: Advanced *In-situ* TEM Workflows Under Reactive Gas Environments

Mark Riccio[1] and Lee Casalena[1]

[1]Thermo Fisher Scientific, Hillsboro, OR 97124

Understanding gas–solid interactions at the atomic scale is essential for the design of new catalysts, energy conversion materials, and nanostructured devices. Recent advances in environmental transmission electron microscopy (ETEM) now enable unprecedented windowless *in-situ* imaging and spectroscopy capabilities under reactive gas atmospheres at elevated temperatures and pressures beyond 2000 Pa. New generations of ETEM instruments integrate high-stability, aberration-corrected optics with four-stage differentially pumped objective lenses, allowing for atomic-resolution imaging and diffraction during real-time chemical reactions. These systems support flexible high-tilt geometries for 3D analysis, compatibility with *in-situ* heating and cooling holders, and precise environmental control, making it possible to observe structural, morphological, and chemical transformations of functional nanomaterials as they occur.

Crucially, these workflows are now enhanced by developments in integrated electron energy-loss spectroscopy (EELS), complemented by novel multi-channel detectors, and synchronized beam modulation tools. Multi-EELS spectral acquisition with real-time chromatic defocus correction provides enhanced energy resolution, even during dynamic experiments, while pulsed beam illumination and live voltage optimization reduce damage to beam-sensitive samples. These capabilities have been applied across a range of studies, from mapping oxidation states in working catalysts to observing sintering, coke formation, and facet evolution during catalytic cycles. By combining time-resolved imaging with compositional and electronic analysis under near-*operando* conditions, these advanced *in-situ* TEM workflows are accelerating discoveries in heterogeneous catalysis, fuel reforming, environmental remediation, and energy storage materials.

A-87

Towards *In-situ* ASAXS: A Microfluidic System for Real-time Characterization of Nanoparticles in Flow

Jiajun Tian[1] and Mrinal Kanti Bera[1]

[1]University of Chicago, NSF's ChemMatCARS, Pritzker School of Molecular Engineering, Chicago, IL 60439

Microfluidic devices are widely used in applications such as drug delivery, nanoparticle synthesis, and cell culture. Under steady flow conditions, these devices provide a unique platform for time-resolved observations of nanoparticle reactions and assembly in flow with a subtle time resolution well-tuned by flow rate. By tracking real-time nanoparticle concentration, the dynamics information such as diffusivity of molecules or nanoparticles in flow can be obtained [1,2].

In this study, a microfluidic system was developed for *in-situ* monitoring of nanoparticle assembly and reactions on a microsecond timescale. Using this system, the diffusivity of Brilliant Blue dye solutions was investigated under controlled mixing within the microfluidic channel. To support the analysis, computational fluid dynamics simulations were performed to characterize the flow conditions. Our results indicate that the diffusion coefficient of Brilliant Blue in the solvent is concentration-dependent, and shear-induced diffusion effects were also observed. Furthermore, an automated data collection and analysis pipeline was developed to enable high-throughput measurements under varying flow conditions, with integrated post-processing capabilities.

NSF's ChemMatCARS, Sector 15 at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) is supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1834750 and NSF/CHE-2335833. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

[1] Yates, Emma V., et al. "Latent analysis of unmodified biomolecules and their complexes in solution with attomole detection sensitivity." *Nature chemistry* 7.10 (2015): 802-809.
[2] Aminian, Manuchehr, et al. "The diffusion of passive tracers in laminar shear flow." *Journal of Visualized Experiments: JoVE* 135 (2018): 57205.

One Year without VME: Experience with Galil DMC-4183 Motor Controllers

M. L. Rivers[1]

[1]Center for Advanced Radiation Sources (CARS), The University of Chicago, Chicago,
IL 60637

During the APS dark year, GSECARS (sector 13) replaced all VME hardware. The OMS-58 and MAXv motor controllers were replaced with Galil DMC-4183 motor controllers. The average cost is 5 times less than the new ACS motion controllers that have been used on new APS beamlines. They have advanced functions such as complex coordinated motion, support for absolute BISS encoders, programmable limit switch behavior, and software control of motor current and microstepping.

We are using the following versions of this Galil controller.

DMC-4183-D4140-D4140. ($3,500)
- On-board 3.0A microstepper drivers.
- 64 microsteps/s
- We have 30 of this model configured for Step/Direction output to existing Step-Pak and Phytron drivers. These use RJ-45 connectors to the external drivers.
- We have 6 of this model configured to directly drive larger stepper motors. They use Elco connectors for compatibility with Step-Paks.
- We may eliminate the Step-Paks in the future and use the on-board drivers.

DMC-4183-D4040-D4040. ($2,600)
- On-board 1.4 microstepper drivers.
- 1,2,4,16 microsteps/s
- We have 11 of this model configured directly driving small stepper motors.
- They replace the CARS BP-8000 boxes previously used with OMS controllers and use Elco connectors.

DMC-4183-D3140-D4040. ($2,800)
- 4 channels with on-board 1.4 microstepper drivers.
- 4 channels with on-board 1.0 amp servo drivers for small DC motors
- 1,2,4,16 microsteps/s
- We have 3 of this model configured directly driving both small stepper motors and small servo motors.
- Elco or DB-25 for stepper motors, DB-25 connectors for servo motors.
- They replace Newport XPS controllers.

DMC-4183-D3547-D3547. ($5,300)
- Stepper motors up to 6A/phase, 256 microsteps/s
- 3-phase brushless motors, 8A/phase
- 2-phase brushless motors, 8A/phase
- 1-phase brushed motors, 8A

- We have 2 of this model configured directly driving any type of motor.

We have also upgraded the control system at APS 6-BM-B station to use these Galil controllers. We have had one hardware issue with the Galil controllers where the last 4 channels occasionally output extra pulses and reverse direction incorrectly. Galil is actively working on this issue.

MATERIALS SCIENCE

C-30	Adhikari, Hari
A-31	Barbosa Martins, Jessica
ESRP-32	Carmel Catholic High School
C-33	Fang, Qichen
C-34	Giri, Prakash
A-35	Haddad, Marwan
A-36	Lee, PeiTzu
C-37	Li, Zhiyuan
ESRP-38	Lincoln-Way East High School
A-39	Lorenzo Martin, Maria Cinta
A-40	Majumder, Supriyo
A-41	McCourt, Joseph
A-42	Mumm, Kyle
ESRP-43	Neuqua Valley High School
C-44	Raut, Ayush Arun
A-45	Reta, Tadesse Billo
A-46	Riyad, Iftekhar
C-47	Sim, Yeoseon
ESRP-48	West Aurora High School
ESRP-49	Whitney M. Young Magnet High School
C-50	Zhou, Shiyuan

Mechanistic Insights into Elemental Doping in Nickel-based Cathodes for High-energy Lithium-ion Batteries: Solubility and Impact on Safety and Cycling Performance

Hari Adhikari[1,2,3], Jinghao Huang[1], Pallab Barai[2], Joseph A. Libera[2], Yasuo Ito[3], Jianguo Wen[1], and Feng Wang[2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]Applied Materials Division, Argonne National Laboratory, Lemont, IL 60439
[3]Department of Physics Northern Illinois University, Dekalb, IL 60115

Nickel-based layered oxide cathodes have gained significant attention for next-generation lithium-ion batteries (LIBs) due to their high energy density and cost-effectiveness. The increasing Ni content enhances capacity but also introduces challenges such as severe capacity degradation upon cycling and thermal instability under highly-delithiated states. To address these issues, doping strategies have been widely explored [1,2]. High-valence dopants like niobium (Nb) show potential for stabilizing the cathode structure and improving electrochemical cycling and thermal stability [2,3].

This study explores the solubility and incorporation behavior of Nb, and its effect on cycling and thermal stability in Ni-based low-Co and Co-free cathodes. The effects of Nb doping on phase stability, Li/Ni disorder, charge compensation, and cycling performance are systematically investigated through multiscale-correlated characterization using x-ray diffraction, scanning electron microscopy, and transmission electron microscopy. Our results show that Nb is uniformly incorporated into the lattice at doping levels around 1%; higher concentrations result in inhomogeneous distribution due to its solubility limit. Nb promotes the formation of smaller, and more compact primary particles, along with a decrease in intra-secondary particle porosity [4,5]. The impact of Nb doping on micropore formation, lattice expansion, and its correlation with cycling performance will be investigated through modeling as well. These findings are further correlated with electrochemical and thermal analyses to deepen understanding of Nb's role in enhancing the cycling and thermal stability of Ni-based cathodes, contributing to the development of high-performance lithium-ion batteries [6].

[1] Cui, Zehao, et al. "Navigating thermal stability intricacies of high-nickel cathodes for high-energy lithium batteries." *Nature Energy* (2025): 1-12.
[2] Xin, Fengxia, et al. "Importance of High Valence Element Nb in Ni-Rich Layered Cathodes for High-Voltage Lithium-Metal Batteries." *ACS Energy Letters* 9.10 (2024): 5172-5178.
[3] Chen, Ke, et al. "Cobalt-free composite-structured cathodes with lithium-stoichiometry control for sustainable lithium-ion batteries." *Nature Communications* 15.1 (2024): 430.
[4] Park, Geon-Tae, et al. "Introducing high-valence elements into cobalt-free layered cathodes for practical lithium-ion batteries." *Nature Energy* 7.10 (2022): 946-954.
[5] Adhikari, Hari, et al. "Microscopic Insights into How High-Valence Elements Stabilize Nickel-Based Cathodes for High-Energy Batteries." (2025).

Work performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, was supported by the Office of Basic Energy Sciences and the Office of Energy Efficiency and Renewable Energy, both under Contract No. DE-AC02-06CH11357.

A-31

The Role of the Dopant on Electronic Structure of Erbium-doped Oxides for Quantum Memory

J.B. Martins[1], G. Grant[2,3], D. Haskel[1], G. Sterbinski[1] I. Masiulionis[2,3], K. Sautter[2,3], E. Karapetrova[1], S. Guha[2,3], and J.W. Freeland[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Pritzker School of Molecular Engineering, The University of Chicago, Chicago, IL 60637
[3]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439

Quantum communication networks rely on qubits, such as photons, for secure long-distance communication. Rare-earth ion (REI) memory systems, particularly those employing erbium (Er^{3+}) in oxide hosts with C-band emission properties, play a pivotal role in synchronizing entanglement for signal amplification within quantum networks [1,2]. Oxides offer advantages such as growth simplicity, compatibility with complementary metal-oxide-semiconductor (CMOS) technology, and long coherence times. However, embedding Er^{3+} ions introduce defects that perturb the host lattice, leading to variations in photoluminescence linewidths and lifetimes in Er-doped oxide films, the causes of which remain unclear [3,4]. In this study, we utilize cutting-edge synchrotron-based x-ray tools from the Advanced Photon Source, including x-ray absorption spectroscopy and diffraction, to investigate the electronic and crystal structures of Er-doped titanium oxides across varying doping levels [5]. This investigation is essential for understanding and controlling the tunability of excited state lifetimes and rare-earth defect linewidths, thereby mitigating decoherence effects in quantum communication systems.

This work was supported by Q-NEXT, a U.S. Department of Energy Office of Science National Quantum Information Science Research Centers under Award No. DE-FOA-0002253. The use of the Advanced Photon Source, Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1] Zhong, M. et al. Nature, 2015, 517, 177–180.
[2] Kanai S. et al., PNAS, 2022, **119**(15), e2121808119.
[3] Singh, M. K., et al., arXiv, 2022, preprint arXiv:2202.05376.
[4] Phenicie, C.M., et al, NanoLett., 2019, **19**(12): p. 8928-8933.
[5] Martins, J.B., et al, APL Mat., 2024, 12, 121110.

ESRP: Study of Cycling Effects on Molybdenum-based Anodes in Batteries

Sudarshan Luitel[1], Carlo Segre[1], Ainsley De Rosa[2], Kayla Johnston[2], Danielle Susanto[2], and Matthew Zell[2]

[1]Illinois Institute of Technology, Chicago, IL 60616
[2]Carmel Catholic High School, Mundelein, IL 60060

Lithium-ion batteries typically have an anode of graphite, but other elements such as molybdenum trioxide (MoO_3) can be substituted. While molybdenum has a high theoretical capacity of 1117 mAh/g, its application is hindered by its rapid capacity degradation after multiple cycles of the battery. This project investigates the electrochemical performance of MoO_3 through half-cell characterization and explores the underlying degradation mechanisms using ex-situ X-ray Absorption Fine Structure (XAFs) analysis. This research provides insights into the structural and chemical transformations that occur during cycling and sheds light on potential failure modes and pathways for the performance enhancement of MoO_3.

C-33

Lightweight Silver-carbon Nanotube Fiber Conductors for Enhancing Electric Power Transmission

Qichen Fang[1], Han Tran[1], Ayush Raut[2], and Vesselin Shanov[1, 2]

[1]Department of Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH 45219
[2]Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH 45219

Replacing conventional copper conductors with lightweight, high-performance alternatives is critical to improving energy efficiency in transportation systems [1]. This work demonstrates the development of a scalable silver-carbon nanotube (Ag-CNT) composite fiber for next-generation power transmission cables. Through a multistep fabrication process combining dry spinning with Ag nanoparticles (AgNPs) mist infiltration, densification, and roll to roll surface functionalization along with silver electroplating, we achieved a hybrid conductor with a unique hierarchical structure. The composite exhibits an electrical conductivity of 8.7×10^6 S/m and ampacity of 4.7×10^3 A/cm^2 while maintaining an ultralow density of 0.4 g/cm^3 and tensile strength of 0.3 GPa. A key innovation is the mist infiltration method that uniformly distributes AgNPs within the CNT matrix during spinning, enhancing interfacial contact and electron transport. Comparative analysis shows a 220 times conductivity improvement over pristine CNT fibers and a 95.5% weight reduction per unit length compared to copper cables [2]. These results position Ag-CNT fibers as a transformative solution for automotive and aerospace applications, where reduced cable mass directly translates to lower fuel consumption and CO_2 emissions. The scalable manufacturing approach underscores the potential for industrial adoption of this sustainable technology.

[1] Joseph, Kavitha Mulackampilly, Kyle Brittingham, Vamsi Krishna Reddy Kondapalli, Mahnoosh Khosravifar, Ayush Arun Raut, Brett David Karsten, Hunter J. Kasparian et al. "Lightweight copper–carbon nanotube core–shell composite fiber for power cable application." C 9, no. 2 (2023): 43.
[2] Brillo, J., and Ivan Egry. "Density determination of liquid copper, nickel, and their alloys." *International journal of thermophysics* 24 (2003): 1155-1170.

Synthesis of CNT-hybrid Fabrics for Multifunctional Applications

Prakash Giri[1], Wei-Cheng Hung[1], and Mark J Schulz[1]

[1]Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH 45221

The Floating Catalyst Chemical Vapor Deposition (FCCVD) method is being utilized at the University of Cincinnati's Nanoworld Laboratories for the large-scale synthesis of carbon nanotube (CNT)-based materials. Given the multifunctional nature of CNT-based materials, they have found extensive applications in diverse fields, including nanoelectronics, nanocomposites, energy and hydrogen storage, biomedicine, wearable electronics, smart materials and sensors, air and water filtration, and drug delivery [1-2]. The scalability of the FCCVD approach offers a pathway to transitioning these nanoscale innovations to industrial-scale production, thereby bridging the gap between academic research and commercial applications. Furthermore, our research focuses on the one-step synthesis of CNT-silicone and Kevlar-based fabrics, incorporating nanomaterial additives for advanced applications such as firefighter apparel, conductive and smart structures, radiation protection, and electromagnetic interference (EMI) shielding. Our approach aims to develop next-generation materials with enhanced performance, durability, and adaptability for real-world use.

This work was partially supported by the National Institute for Occupational Safety and Health through the Pilot Research Project Training Program of the University of Cincinnati Education and Research Center Grant T42OH008432, and University of Cincinnati Armstrong Institute for Space, Technology, and Research.

[1] P. Giri, V. K. R. Kondapalli, K. M. Joseph, V. Shanov, M. Schulz, *Nanomater. Basel Switz.* 2023, *13*, 2728.
[2] S. K. Soni, B. Thomas, V. R. Kar, *Mater. Today Commun.* 2020, *25*, 101546.
[3] M. F. L. De Volder, S. H. Tawfick, R. H. Baughman, A. J. Hart, *Science* 2013, *339*, 535.

Process-structure Relationships in Laser Directed Energy Deposition of Molybdenum Powder within a Ti-6Al-4V Matrix

Marwan Haddad[1], Mathew Cohen[2], Aslan Bafahm Alamdari[1], Brian Welk[2], Kamel Fezzaa[3], and Sarah Wolff[1]

[1]Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210
[2]Department of Materials Science and Engineering, The Ohio State University, Columbus, OH 43210
[3]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

Laser directed energy deposition (L-DED) of multi-materials is capable of additively fabricating parts with enhanced properties for biomedical and aerospace applications. This study focuses on the multi-material printing of Ti-6Al-4V (Ti64) and molybdenum (Mo) with L-DED. Alloying Mo with Ti64 improves the high-temperature mechanical properties of Ti64. However, the dynamic and melting behavior of the Mo powder inside the Ti64 matrix and their impact on the L-DED process and the microstructure are still unclear. This study utilizes *in-situ* monitoring techniques, namely high-speed x-ray imaging and infrared imaging, with post-process material characterization techniques to relate the L-DED process of depositing Mo powder onto a Ti64 matrix to the final microstructure. Results showed Mo powder particles motion inside the melt pool were governed by the convective fluid flow. The convective fluid flow achieved an overall homogeneous macro-scale chemical composition by influencing the melting behavior of Mo powder particles and contributing to the liquid mixing. The increase of Mo content in Ti64 did not impact the melt pool temperature. Lastly, Mo segregated at the micro-scale near the top surface, and Mo-rich regions were located near un-melted powder particles in the final build. This work can help in improving future work on multi-material applications and verify simulation models for L-DED.

National Science Foundation (NSF) grant CMMI-2245141 supported this work. The authors would like to thank Tao Sun, Niranjan Parab, Alex Deriy, and Benjamin Gould who helped conduct the experiment at the 32-ID-B beamline at the Advanced Photon Source (APS), which is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory (ANL) under Contract No. DE-AC02-06CH11357 and supported through Laboratory Directed Research and Development (LDRD) funding from ANL under the same contract. In addition, the authors would also like to thank Sizhe Xu, Kristina May, and Jianyue Zhang from the Ohio State University, Sarah Mikula and Daniel Veghte from the Center for Electron Microscopy and Analysis (CEMAS), Hui Wang from Texas AM Engineering Experiment Station (TEES), and Samuel Clark from APS.

A Simulation Study of Self-absorption in Synchrotron X-ray Fluorescence

Pei-Tzu Lee[1], Yi Jiang[1], and Olga Antipova[1]

[1]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

Synchrotron x-ray fluorescence (XRF), especially when combined with 2D and 3D tomographic methods, is a powerful technique for materials analysis. However, the accuracy of XRF data can be undermined by self-absorption, where fluorescence photons are attenuated within the sample before detection, thereby skewing quantitative results. In this study, we present a combined simulation and experimental approach to investigate and correct for self-absorption effects in synchrotron XRF measurements. We employ a simulation framework that incorporates realistic beam properties, sample geometries, and detection setups to model the impact of self-absorption under various experimental conditions. The simulations are validated with experimental data acquired at beamline 2-ID-E of the Advanced Photon Source (APS). By systematically varying incident beam energy, sample thickness, and acquisition geometries—especially in both 2D and 3D tomographic configurations—we elucidate how self-absorption manifests and propose strategies for its mitigation. Our findings provide practical guidelines for optimizing synchrotron XRF experiments, reducing errors introduced by self-absorption, and enhancing the reliability of elemental mapping. These insights are broadly applicable to research areas such as materials science, environmental analysis, and bio sample research, where precise quantification of elemental distributions is critical.

Semi-dry Roll-to-roll Printing of Electrodes for Lithium-ion Batteries

Zhiyuan Li[1] and Tao Sun[1]

[1]Department of Mechanical Engineering, Northwestern University, Evanston, IL 60208

The increasing demand for secondary energy storage in various industries facilitates advancements in lithium-ion batteries (LIBs). However, progress in LIB manufacturing lags behind material innovations [1]. The state-of-the-art wet slurry process for electrode manufacturing suffers from solvent toxicity, high cost, and electrode microstructural limitations [2]. Recently, several solvent-free dry electrode manufacturing technologies such as dry electrostatic spraying, Maxwell-type dry coating, and hot pressing have emerged, aiming to reduce manufacturing footprint, cost, and energy consumption. Nonetheless, these dry electrode technologies face material and processing challenges that hinder their industrial application. Examples include limited selection of binder materials, inhomogeneous feedstock mixing, difficult quality monitoring, and weak adhesion due to non-uniform binder distribution [3,4].

Here, we propose an eco-friendly, semi-dry roll-to-roll process assisted by aqueous inkjet printing with the potential for integration into existing wet electrode production lines and the ability to overcome the limitations of dry electrode technology. We summarize the basic steps of the feedstock preparation, ink rheology formulation, and the resulting electrode structure and properties of a $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ cathode. We report a unique electrode architecture with a porosity gradient beneficial to fast charging performance. We plan to utilize synchrotron x-ray nano-tomography paired with high fidelity multi-physics models to reveal the microstructural advantages of the printed electrode over the conventional wet slurry electrode. We further plan to combine *operando* transmission x-ray microscopy (TXM) with x-ray absorption near edge spectroscopy (XANES) to probe the rate-dependent phase change inhomogeneity in printed versus wet electrodes.

[1] Liu, Y., Zhang, R., Wang, J., & Wang, Y. (2021). Current and future lithium-ion battery manufacturing. *IScience*, *24*(4), 102332. https://doi.org/10.1016/j.isci.2021.102332
[2] Lu, Y., Zhao, C.-Z., Yuan, H., Hu, J.-K., Huang, J.-Q., & Zhang, Q. (2022). Dry electrode technology, the rising star in solid-state battery industrialization. *Matter*, *5*(3), 876–898. https://doi.org/10.1016/j.matt.2022.01.011
[3] Kim, N.-Y., Kim, J.-H., Koo, H., Oh, J., Pang, J.-H., Kang, K.-D., Chae, S.-S., Lim, J., Nam, K. W., & Lee, S.-Y. (2024). Material Challenges Facing Scalable Dry-Processable Battery Electrodes. *ACS Energy Letters*, *9*(11), 5688–5703. https://doi.org/10.1021/acsenergylett.4c01690
[4] Tao, R., Gu, Y., Du, Z., Lyu, X., & Li, J. (2025). Advanced electrode processing for lithium-ion battery manufacturing. *Nature Reviews Clean Technology*, *1*(2), 116–131. https://doi.org/10.1038/s44359-024-00018-w

ESRP: Creating a Ti02 Thin Film on Variable Substrates Using Solid Phase Epitaxy

Rui Liu[1], Benjaman Voliva[2], Griffin Reidy[2], Alexander Lizak[2], Joshua Dare[2], Tyler Fox[2], Jenna Abuhamdan[2], Ishaan Patel[2], Peyton Komer[2], and Damilola Alabi[2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]Lincoln Way East, Frankfort, IL 60423

In the past years there has been a growing excitement for quantum computers, their use cases, and the development of them. The unparalleled processing power and security that results from computing in a quantum state rather than a binary state makes way for endless possibilities of systems that can compute with many more variables than would be realistic for typical computers. The challenge that arises for those who set out to build quantum chips is in the creation of thin films that can hold information in a quantum state. This is due to specific crystalline structure that fosters the ability for quantum tunneling with decreased decoherence. In this study we set out to create one of these thin films out of TiO2 onto substrates made of Silicon and Sapphire respectively using the process of Solid Phase Epitaxy. TiO2 was chosen due to its telecom-band optical transition at 1.54 micrometers; long optical and spin coherence times; and compatibility with integrated photonic platforms. These substrates would have the opportunity for a predetermined geometry to eliminate the need for etching and will depose via the atomic layer method to limit the potential for impurities. After synthesizing the thin films, half of each substrate went untouched while the other went through an intense annealing process of 800 degrees Celsius for 10 hours to reclaim its crystalline structure. We then characterized these films using atomic force microscopy (AFM) for surface morphology, x-ray reflectivity (XRR) for thickness, density, and roughness, and x-ray diffractions for crystallographic analysis. After doing this characterization we were able to conclude that there is an immense difference in structure between substrate materials due to what we believe is a difference in each material's lattice structure. This was evident in TiO2 crystal sizes being up to 10x bigger in silicon in comparison to sapphire. It also became evident atomic layer deposition was a valuable method in creating an amorphous film; however, to create the desired crystal structure an annealing process was vital. These results make evident the idea that TiO2 is a valuable material for quantum computing in concurrence with an optimized substrate.

Synchrotron *In-situ* Study of Scuffing Evolution

Farida Ahmed Koly[1], David L. Burris[1], Stephen Berkebile[2], Nikhil Murthy[2], Scott Walck[2], Cinta Lorenzo Martin[3], Oyelayo Ajayi[3], Peter Kenesei[4], and Jun-Sang Park[4]

[1]University of Delaware, Newark, DE 19716
[2]U.S. Army Combat Capabilities Development Command Army Research Laboratory, Adelphi, MD 20783
[3]Applied Materials Division, Argonne National Laboratory, Lemont, IL 60439
[4]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

Scuffing, a type of surface damage in highly stressed and poorly lubricated sliding contacts, is characterized by a rapid increase in friction and severe plastic deformation of the near surface material. Scuffing is difficult to study directly due to a lack of access to the contact interface and the speed of failure. This talk presents real-time characterization of scuffing failure of lubricated steel in a reciprocating contact using high-energy, high-speed synchrotron x-ray diffractometry. *In-situ* XRD of the contact interface during scuffing showed a sharp increase in the peak FWHM, which is attributed to grain refinement and increase in dislocation density. Additionally, *ex-situ* experiments consisting of 1-micron step XRD depth profile before and after scuffing showed a reversal and enhancement of a sinusoidal strain pattern of the near-surface region with localized tension in the loading and compression in the sliding directions after scuffing.

A Non-destructive Approach for Probing the Atomic-scale Interface Structure of Supported 2D Transition Metal Dichalcogenide Semiconductors

S. Majumder[1], N. Shinde[2], J. Cavin[3], C. Chen[4], A. B. Dey[5], K. V. L. V. Narayanachari[1], J. Zhang[1], D. A. Garcia-Wetten[1], O. Dieguez[2], S. Hettler[6], A. Cohen,[2] D. T. Keane[1], R. Arenal[6], J. M. Rondinelli[1], A. Ismach[2], and M. J. Bedzyk[1]

[1]Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208
[2]Department of Materials Science and Engineering, Tel Aviv University, Ramat Aviv, Tel Aviv 6997801, Israel
[3]Department of Mechanical Engineering and Material Science, Washington University in St. Louis, St. Louis, MO 63130
[4]2D Crystal Consortium - Materials Innovation Platform, Materials Research Institute, The Pennsylvania State University, University Park, PA 16802
[5]Deutsches Elektronen-Synchrotron DESY, Hamburg 22607, Germany
[6]Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, 50018 Zaragoza, Spain

In the 2D materials family, transition metal dichalcogenides (TMDs) possess tuneable bandgaps and controllable surface mobilities favorable for optoelectronics, flexible solid-state devices, field-effect transistors, ultrasensitive sensors, and efficient energy conversion applications [1]. The surface termination of the underlying support and reconstruction at the support-over-layer interface plays a significant role in the functional aspects of the 2D system. Knowledge of such a buried interface structure, atomically and chemically, is crucial to understanding its impact on electronic and optical properties. In this regard, commonly used scanning probe microscopy is only partly beneficial since the buried interface is not directly observable via this top-down method, and electron microscopy requires a cross-sectional preparation that can severely modify the delicate vdW interfaces. Our recent work employs a novel combination of synchrotron x-ray scattering and spectroscopy techniques in a relatively non-destructive way to produce a highly resolved chemically sensitive atomic profile for the substrate terminal layer, interface bilayer, and 2D nanocrystal layer. We are developing a global structural analysis strategy for different length scales to produce the interfacial map with sub-Å resolution. This allows us to correlate how different MOCVD recipes lead to changes in chemical and structural terminations of the supporting substrate surface, which hugely affect the subsequent 2D WS_2 crystal growth in terms of their lateral domain sizes, vdW gaps, epitaxial registry, and stability. These studies can provide general insight into the structure-property relationships of vdW heteroepitaxial systems relevant to nano-electronic, optoelectronic, and energy conversion applications.

Part of this work uses the 5ID-C DNDCAT beamline at the Advanced Photon Source (APS), an Office of Science User Facility operated for DOE by Argonne National Laboratory, supported by DOE under Contract DE-AC0206CH11357.

[1] Choi, W.; Choudhary, N.; Han, G. H.; Park, J.; Akinwande, D.; Lee, Y. H. Recent development of two-dimensional transition metal dichalcogenides and their applications. *Mater Today* 2017, *20* (3), 116-130. DOI: 10.1016/j.mattod.2016.10.002.

Pty-co-SAXS: Combining Ptychography and Small-angle X-ray Scattering for Nanostructure Characterization

Joseph McCourt[1], Junjing Deng[1], Byeongdu Lee[1], Seonke Seifert[1], Mathew Cherukara[2], Hemant Sharma[2], Ming Du[2], Zhihua Cheng[3], Boyu Zhang[4], and Matthew Jones[5]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Computational Science and Artificial Intelligence, Argonne National Laboratory, Lemont, IL 60439
[3]Department of Chemistry, Northwestern University, Evanston, IL 60208
[4]Department of Mechanical Engineering, Northwestern University, Evanston, IL 60208
[5]Department of Chemistry, Rice University, Houston, TX 77005

Multi-length scale characterization is crucial for hierarchical materials, as nanostructure morphology and local arrangements influence material properties. While small-angle x-ray scattering (SAXS) provides valuable structural insights, its ensemble-averaged data limits the understanding of local variations. X-ray ptychography, a coherent diffraction imaging technique, offers high-resolution imaging of internal structures, making it an ideal complement to SAXS. This combined approach, pty-co-SAXS, enables nanoscale morphological mapping alongside reciprocal-space information on nanostructure size, shape, and orientation. The upgraded Advanced Photon Source will significantly enhance ptychography and SAXS capabilities through increased coherent flux. This work demonstrates how integrating both techniques within a single sample environment and detector setup can optimize data correlation while minimizing radiation dose.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility and is based on work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. DOE under Contract No. DE-AC02-06CH11357.

Synchrotron X-ray Methods for Laser Powder Bed Fusion: Imaging and Diffraction Contributions to the IMQCAM Digital Twin

Kyle Mumm[1], Jiayun Shao[1], and Tao Sun[1]

[1]Department of Mechanical Engineering, Northwestern University, Evanston, IL 60208

While Laser Powder Bed Fusion (LPBF) has established itself as a complex and versatile metal manufacturing technique, the mechanical properties of the resulting prints are often undermined by embedded defects. Accordingly, qualification and certification (Q&C) is a critical step in the application of LPBF-manufactured parts, but the wide potential variation between identically manufactured parts complicates the process significantly. To replace current methods such as x-ray computed tomography, the NASA Institute for Model-based Qualification and Certification of Additive Manufacturing (IMQCAM) resolves to create a digital twin that serves as a suitable surrogate for a printed asset, reducing the testing burden and acting as a viable surrogate for the purposes of Q&C [1].

Using the high-speed imaging and diffraction techniques at the Advanced Photon Source, our team offers contributions to the modeling efforts that aim to predict the defect size, quantity, and location, as well as to predict the microstructure in response to printing conditions and heat treatments. Our work on the defect model focuses on stochastic porosity, such as that created by spattered metal interfering with the laser melting process. Using high-speed *operando* x-ray imaging data from the 32-ID beamline, we investigate the spattering rate, size, and its relationship to the melting state. This enables us to build a comprehensive and physics-informed statistical model for stochastic spatter-related defects, which aids the greater defect model's prediction of more deterministic defects. Simultaneously, we assist the microstructure model by providing minor phase quantification of IN718 through high-energy x-ray diffraction experiments at the 1-ID beamline. While as-printed bulk geometries pose difficulties for diffraction experiments, primarily due to the large grain sizes and texture, we will collaborate with Dr. Ping Guo's team at Northwestern University to generate powder with ultrasonic vibration machining, enabling future experiments to contrast the bulk samples against the generated powder [2].

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory, as well as support from a NASA Science Technology Research Institute under Grant Number 80NSSC23K1342.

[1] Institute for Model-based Qualification and Certification of Additive Manufacturing, https://www.imqcam.org/
[2] Wang, Yaoke, et al. *Additive Manufacturing* 81 (2024): 103993.

ESRP: X-ray Diffraction Analysis of Prosthetic Materials

Fiona Lin[1], Adrian Martinez[1], Jonathan Ostendorf[1], Daria Prawlocki[1], Andrea Ramirez[1], Valeria Ramirez[1], Milan Shah[1], Advaitha Taire[1], Denis T. Keane[2], and Joseph Kopke[3]

[1]Neuqua Valley High School, Naperville, IL 60564
[2]DND-CAT, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[3]Northwestern University Prosthetic and Orthotic Center, Chicago, IL 60611

Prosthetic and orthotic research involves various materials to consider relating to strength, flexibility and durability. By utilizing x-ray fluorescence, the comparison of two orthotic material samples before and after application of strain can be examined through spectroscopy. The two materials that will be examined under spectroscopy are Acrylonitrile Styrene Acrylate (ASA) and Nylon Carbon Fiber. The resulting composition of the materials before and after application of strain will be studied using XAFS. Results for each material will be compared to further understand the structure of each material before and after strain.

Thanks to Kelly Sturner from the Exemplary Student Research Program and Dr. Denis Keane, Dr. Qing Ma, and Mr. William Guise from DND-CAT. This research was made possible through the Exemplary Student Research Program, supported by Argonne National Laboratory's Educational Programs (CEP), the APS User Office, Neuqua Valley teacher, Daria Prawlocki, NUPOC, Joseph Kopke and supported by the use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, and was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357. We are grateful for the use of sector 5 DND-CAT facilities at the APS which are operated by DuPont, Northwestern University, and Dow. Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

Strategies to Dope 3D Graphene for Flexible Thermoelectric Applications

Ayush Arun Raut[1], Vamsi Krishna Reddy Kondapalli[1], and Vesselin Shanov[2]

[1]Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH 45221
[2]Department of Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH 45221

This study explores innovative strategies to dope three-dimensional graphene sheet (3DGS) for flexible thermoelectric (TE) applications. By employing various p-type and n-type doping methods, significant improvements in electrical conductivity and Seebeck coefficient were achieved. Chemical doping, polymer doping, and atomic nitrogen and oxygen addition via techniques such as dip coating, hydrothermal technique, drop casting, and thermal annealing were utilized to develop p-doped and n-doped 3DGS [1].

Characterization techniques including SEM, TEM, Raman spectroscopy, and XPS confirmed the structural integrity and doping efficacy. The doped 3DGS exhibited notable enhancements in electrical conductivity and Seebeck coefficient. The best-performing n-type samples reached electrical conductivities up to 53.86 S/cm and Seebeck coefficients as high as -44.3 μV/K, while p-type samples achieved an electrical conductivity of 13.4 S/cm and Seebeck coefficients up to 35.25 μV/K. Furthermore, a flexible TE device developed from these materials demonstrated an internal resistance of 42.89 Ω, the estimated maximum power output for ~17K temperature difference was approximately 24.5 μW, corresponding to a power density of 12.25 mW/cm^2 [1]. These findings highlight the potential of 3DGS as a versatile material for energy harvesting and sensing applications, paving the way for the development of efficient, flexible, and sustainable energy solutions for wearable electronics and the Internet of Things (IoT) [2, 3].

[1] Ayush Arun Raut, 1, VKRK, , Yu Zhang, NR, BLK, 2, Ryan James Chapman, 3, HT, OIA, Je-Hyeong Bahk, aVS, 4. Strategies to dope 3D graphene for flexible thermoelectric applications. In press.
[2] Hsieh Y, Zhang Y, Zhang L, Fang Y, Kanakaraaj SN, Bahk J, Shanov V. High thermoelectric power-factor composites based on flexible three-dimensional graphene and polyaniline. *Nanoscale.* 2019 Apr 4; 11(14): 6552–6560. PMCID:30916066; 10.1039/C8NR10537E.
[3] Du Y, Xu J, Paul B, Eklund P. Flexible thermoelectric materials and devices. *Applied materials today.* 2018 Sep 1; 12: 366–388. PMCID:10.1016/j.apmt.2018.07.004.

In-situ Synchrotron X-ray Studies of Epitaxial SrCoOx Heterostructures

Tadesse Billo Reta[1], Yan Li[1], Qingteng Zhang[2], Eric M. Dufresne[2], Hua Zhou[2], and Dillon D. Fong[1]

[1]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

The reversible topotactic phase transition in strontium cobaltite ($SrCoO_x$) thin films, controlled by oxygen stoichiometry, holds significant potential for neuromorphic and ionotronic devices. Here transition between the brownmillerite (BM) $SrCoO_{2.5}$, an insulating antiferromagnet, and the perovskite (PV) $SrCoO_3$, a ferromagnetic metal, can be precisely manipulated by varying the oxygen concentration. Despite extensive research into their magnetic and electronic properties, the kinetics and dynamics of oxygen vacancy ordering under different thermal and environmental conditions remain inadequately understood.

In this study, we utilize *in-situ* coherent x-ray scattering at the Advanced Photon Source to monitor the phase evolution and vacancy dynamics of epitaxial $SrCoO_x$ thin films grown on $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}(001)$ (LSAT) substrates under alternating O_2 and N_2 atmospheres. We study the kinetics of the phase transition from 300ºC to 360ºC, noting distinct behaviors when switching between oxidized and reduced phases. The vacancy ordering kinetics are compared to X-ray Absorption Near Edge Structure (XANES) measurements conducted at the Co K-edge, demonstrating the distinction between oxygen vacancy injection and vacancy ordering. We compare our results with those from films grown on $SrTiO_3$ (STO) substrates, illustrating the influence of epitaxial strain on the phase transition.

This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under contract number DE-AC02-06CH11357.

Developing an Efficient Crystal Plasticity Finite Element Simulation Workflow to Guide *In-situ* Grain-resolving X-ray Imaging

Iftekhar A. Riyad[1], Jun-Sang Park[1], Seunghee Oh[1], Hemant Sharma[1], Sinisa Veseli[1], Tejas Guruswamy[1], Mark C. Messner[2], Xuan Zhang[3], and Stephan O. Hruszkewycz[4]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Applied Materials Division, Argonne National Laboratory, Lemont, IL 60439
[3]Nuclear Science Engineering Division, Argonne National Laboratory, Lemont, IL 60439
[4]Materials Science and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

This study is concerned with developing an efficient crystal plasticity finite element (CP-FE) simulation workflow designed to use 3D grain map acquired from *in-situ* high-energy diffraction microscopy (HEDM) experiment. The workflow will facilitate identification of grains of interest (GOIs) so that they can be investigated with higher-resolution x-ray imaging techniques. In this workflow, a digital twin of the polycrystalline material measured by far-field (FF) and/or near-field (NF) HEDM is generated using a combination of DREAM3D [1] and Cubit/Sculpt [2]. Multi-physics Object-Oriented Simulation Environment (MOOSE) [3] is used as the finite element solver, and New Engineering Material Modeling Library (NEML2) [4] is used to describe the CP deformation mechanism. This simulation workflow will utilize ALCF Polaris to provide real-time guidance to *in-situ* deformation experiment of polycrystalline sample at the High Energy X-ray Microscope (HEXM) beamline of the Advanced Photon Source (APS) at Argonne National Laboratory (ANL), an APS-U feature beamline capable of imaging polycrystalline materials at the meso- and nanoscales in a single instrument. The ability to effectively identify GOIs through real-time digital twin simulations will allow users to fully exploit the zoom-in and zoom-out capabilities of HEXM and test hypotheses relevant to understanding the structure-property-process relationship.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility and is based on work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. DOE under Contract No. DE-AC02-06CH11357.

[1] Groeber, M.A. and M.A. Jackson, *DREAM.3D: A Digital Representation Environment for the Analysis of Microstructure in 3D.* Integrating Materials and Manufacturing Innovation, 2014. 3(1): p. 56-72.
[2] Blacker, T.D., W.J. Bohnhoff, and T.L. Edwards, *CUBIT mesh generation environment. Volume 1: Users manual*. 1994, Sandia National Lab.(SNL-NM), Albuquerque, NM (United States).
[3] Icenhour, C., et al., *Multi-physics object oriented simulation environment (moose)*. 2018, Idaho National Lab.(INL), Idaho Falls, ID (United States).
[4] Hu, T., et al., *NEML2: A High Performance Library for Constitutive Modeling*. 2024, Argonne National Laboratory (ANL), Argonne, IL (United States); Idaho.

Design for PFAS-free High-loading Electrode in Li-ion Batteries

Yeoseon Sim[1,2], Jihyeon Gim[3], Eungje Lee[3], and Elena Shevchenko[1]

[1]Department of Materials Science Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea
[2]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[3]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

The development of thick electrodes is essential for advancing high-energy-density lithium-ion batteries (LIBs) in limited spaces by maximizing active material loading and minimizing the passive fraction [1]. However, their increased thickness leads to challenges in mechanical integrity, sluggish ionic transport, and poor electronic conductivity that must be addressed to enable practical application [2]. In this study, we designed a flexible high-loading (up to ~15 mg cm^{-2}) electrode by integrating Li- and Mn-rich layered oxides (LMR) particles with a lightweight multiwalled carbon nanotubes (MWCNTs with 100 μm length) through Per- and polyfluoroalkyl substances (PFAS)-free and N-Methyl-2-pyrrolidone (NMP)-free process. The designed electrodes demonstrate a comparable specific capacity and initial columbic efficiency to conventional slurry-coated electrodes (SCE, ~13.2 mg cm^{-2} on 20 μm Al foil) and revealed improved stability and rate capability. These improvements are attributed to the outstanding chemical durability and high porosity of electrode architecture without the use of polymeric binder. Notably, our electrode, prepared with a higher loading compared to the SCE, achieved a 36% increase in electrode-level gravimetric capacity and a 42% increase in volumetric capacity. This sustainable, lightweight electrode design offers a promising eco-friendly platform for development of high-loading electrodes across a wide range of electrochemically active materials.

This research was supported by the Basic Science Research Program (RS-2024-00346374) through the National Research Foundation (NRF) of Korea funded by the Ministry of Science and ICT. Work performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, was supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1] Jianlin Li et al. From Materials to Cell: State-of-the-Art and prospective Technologies for Lithium-Ion Battery Electrode Processing. *Chem. Rev*. 2022, 122, 903-956
[2] Arturo Gutierrez et al. Review-Earth-Abundant, Mn-rich Cathodes for Vehicle Applications and Beyond: Overview of Critical Barriers. *J. Electrochem. Soc*. 2023, 170, 030509

ESRP-48

ESRP: Ruby Microwave Fabrication

Ben Diroll[1], Jacob R. Wadle[2], Linnae Ellis[2], Chase Ferreiro[2], David Alcantar[2], Dylan Raskosky[2], Julie Zaborac[3], and Sandy Scott[3]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]West Aurora High School, Aurora, IL 60506
[3]Science Department, West Aurora High School, Aurora, IL 60506

Last year, West Aurora High School students used iron wool to maximize ruby growth, but their chromium (III) oxide and aluminum oxide ratios were inconsistent. This year, we used a paperclip as a catalyst, predicting its uniform shape would centralize the metal-nonmetal reaction and yield larger, more concentrated rubies. We also hypothesized that rubies would form on the crucible surfaces, allowing us to analyze how surface orientation affects ruby shape.

Studies show that the reaction between aluminum oxide and chromium (III) oxide procurers a brighter red pigmentation and a more concentrated reaction through the use "small number of aluminum atoms being replaced by chromium atoms [1 in 5000]," so this year we are opting to test with smaller amounts of chromium in relation to aluminum in comparison to the previous years’ more sporadic ratios [1].

We conducted trials in a 50 mL crucible, varying paper clip placement. Last year, two of nine samples showed promising ruby characteristics. This year, we aimed for larger, more consistent rubies while assessing catalyst positioning effects. Standardizing trials was crucial, and we expanded on the most successful sample by testing X, Y, and Z-axis paperclip placements. To analyze our results, we employed fluorescence testing, x-ray diffraction, SEM, and cathodoluminescence.

[1] *Molecular Expressions: The Birthstone Collection - Ruby*. (2025). Fsu.edu. https://micro.magnet.fsu.edu/birthstones/pages/ruby.html

ESRP: Studying Ni_2P and NiCoP as Viable Catalyst Alternatives to Au and Pt in Hydrogen Evolution Reactions

Kavin Ramasamy[1], Mia Resendiz[1], Nithin Ramasamy[1], William Wang[1], Samar Mohan[1], Paras Cherukuri[1], Karina Pena[1], Keith Xin[1], Andrew Peterson[1], Karen Andrea Castañeda Marín[2], and Carlo Segre[2]

[1]Whitney M. Young Magnet High School, Chicago, IL 60607
[2]Illinois Institute of Technology, Chicago, IL 60616

Hydrogen fuel cells are a renewable energy source that extracts energy from water through electrolysis. Using hydrogen as a fuel can have lasting positive effects on the environment by reducing dependence on harmful fossil fuels.

Fuel cells make use of catalysts to help enhance the hydrogen evolution reactions (HER). Discovering efficient and cost-effective catalysts for HER would be revolutionary as the current catalysts - gold (Au) and platinum (Pt) - have high costs that prevent large-scale development. Due to this dilemma, alternative catalysts such as nickel cobalt phosphide (NiCoP) and nickel phosphide (Ni_2P) have attracted attention in HER.

This work presents the study of Ni_2P and NiCoP as catalysts for HER. Structural characterization of the materials was performed using powder x-ray diffraction (XRD) and x-ray absorption spectroscopy (XAS). Linear sweep voltammetry (LSV) was used to evaluate the electrocatalytic activity of the catalysts. Experiments were conducted using a rotating disk electrode (RDE) in a three-electrode cell configuration. The on-set potential of NiCoP was lower than that of Ni_2P, and the current was also superior. This indicates that the bimetallic NiCoP outperforms Ni_2P in terms of both energy efficiency and catalytic activity. The potential of using NiCoP as a cost-effective catalyst remains promising and is a viable option for future catalyst development.

[1] Sun, X., Zhang, H., Liu, M., Wang, J., Xu, H., & Wang, G. (2019). Interface engineering of CoP nanosheets and Ni2P nanoparticles hybrid as an efficient bifunctional electrocatalyst for overall water splitting. *Electrochimica Acta*, *328*, 134798. https://doi.org/10.1016/j.electacta.2019.134798
[2] Li, W., Liu, Y., Wang, Y., Yang, G., & He, D. (2022). Recent Advances in Transition Metal-Based Electrocatalysts for the Hydrogen Evolution Reaction in Alkaline Media. *Advanced Functional Materials*, *32*(40), 2208358. https://doi.org/10.1002/adfm.202208358
[3] Wang, J., Xu, F., Jin, H., Chen, Y., & Wang, Y. (2020). Non-Noble Metal-Based Carbon Composites in Hydrogen Evolution Reaction: Fundamentals to Applications. *ACS Catalysis*, *10*(7), 4190–4204. https://doi.org/10.1021/acscatal.0c02301
[4] Woodford, C. (n.d.). *Fuel cells*. Explain That Stuff. Retrieved April 4, 2025, from https://www.explainthatstuff.com/fuelcells.html
[5] Plug Power. (n.d.). *Fuel cell benefits*. Retrieved April 4, 2025, from https://www.plugpower.com/fuel-cell-power/fuel-cell-benefits/

C-50

Visualizing Interfacial Structure and Reaction Behavior of Li-chalcogen Batteries

Shiyuan Zhou[1], Yuzi Liu[2], Gui-Liang Xu[1], and Khalil Amine[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439
[2]Nanoscience and Technology Division, Argonne National Laboratory, Lemont, IL 60439

Lithium-ion batteries (LIBs) have played a pivotal role in the transition to renewable energy, powering applications from electric vehicles (EVs) to grid-scale energy storage systems. However, the increasing demand for higher energy density and cost-effective battery technologies necessitates the development of next-generation energy storage systems capable of achieving an energy density of 500 Wh kg^{-1} by 2030. Chalcogen elements (O, S, Se, Te) from Group 16 of the periodic table offer unique potential due to their ability to undergo multi-electron transfer reactions and significantly enhancing energy density [1,2]. Despite this promise, Li-chalcogen batteries face critical scientific challenges, including the dissolution and shuttle effect of lithium polyspecies (e.g., polysulfides, polyselenides, and polytellurides), ambiguous reaction pathways, and transient solid-phase intermediates formed during discharge.

Advanced *in-situ/operando* characterization is crucial for understanding these complex mechanisms under realistic operating conditions. However, challenges such as the low atomic number of chalcogen species, beam sensitivity, and low crystallinity hinder precise characterization. Additionally, achieving high spatial and temporal resolution in multimodal imaging remains a fundamental challenge, particularly for tracking the liquid-to-solid conversion of unstable lithium polyspecies. A deeper understanding of the coupled phenomena governing Li-chalcogen batteries—specifically, the dynamic distribution, aggregation, deposition, and dissolution of lithium polyspecies—is urgently needed.

To address these challenges, this work pioneers real-time and cryogenic transmission electron microscopy (TEM) observations of Li-chalcogen reactions [3]. By systematically investigating electron beam effects and optimizing spatiotemporal resolution, a Li-S nanobattery was constructed within a liquid cell, enabling high-resolution visualization of electrochemical transformations at the nano- and atomic scale. This study provides the first real-time imaging of electrochemical interfaces in liquid Li-S batteries. Furthermore, for all-solid-state Li-S batteries, the interfacial structure of Li6PS5Cl||chalcogens was directly visualized.

Through the integration of advanced TEM detectors, unprecedented insights into atomic-scale dynamics, crystal structures, and elemental distributions were achieved. Complementary density functional theory calculations further revealed that concentration-driven aggregation of lithium polyspecies significantly alters their geometric structure, electronic properties, and hybridization orbitals. These findings establish a direct link between lithium polyspecies concentration and reaction mechanisms, which are key factors influencing Li-S battery performance. The elucidated interfacial reaction pathway not only unveils a previously unrecognized transformation mechanism but also deepens the fundamental understanding of Li-S batteries, informing future design strategies for high-energy, long-life, and efficient Li-chalcogen batteries.

[1] Yao W et al. Rechargeable Metal-Sulfur Batteries: Key Materials to Mechanisms. Chemical

Reviews (2024) 124, 4935–5118.
[2] Chen Z & Zhi C. Chalcogens for High-Energy Batteries. Nature Reviews Materials (2025).
[3] Zhou S et al. Nature (2023) 621, 75–81.

NANOSCIENCE & NANOTECHNOLOGY

C-52……………………………………………………………………Boria-Denis, Andrea
C-53…………………………………………………………………………………Jia, Haili
C-54……………………………………………………………………………Jo, Kiyoung
C-55………………………………………………………………………Mao, Yuanbing
C-56…………………………………………………………………McGinn, Christine
A-57……………………………………………………………Zampirolli Leal, Ana Clara
A-58……………………………………………………………………………Zhou, Siyu

C-52

Type II Nonblinking Long-lifetime Giant Colloidal Quantum Dots

Andrea Boria-Denis[1]

[1]University of Illinois at Chicago, Chicago, IL 60607

Semiconductor quantum dots have been increasingly applied in alternative energy and optical applications due to their size dependent properties arising from quantum confinement effects. Current research effort has been applied to increase the lifetime of singly and doubly excited states of bandgap tunable nanomaterials. Previously we reported the development of fully type II giant quantum dots (gQDs) by overcoating gradient alloyed CdZnSe cores with thick CdS shells. Currently, CdSe/ZnSe core systems are under examination, as well as CdZnS/ZnSe gQDs that have achieved radiative lifetimes of over 2 microseconds due to the robust decorrelation between electrons and holes within the core or shell. This new structural motif has resulted in several new applications in lasing and biological imaging and tracking with time gating to reduce biological background fluorescence.

Integrated Computational and Machine Learning Approaches for Atomic-scale Material Characterization

Haili Jia[1], Joseph Smerdon[2], Gi-Hyeok Lee[3], Arthur McCray[4], Samuel D. Marks[5,6], Miaofang Chi[7], Wanli Yang[3], Colin Ophus[5], Haidan Wen[6], Jeffrey Guest[1], and Maria Chan[1]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]Jeremiah Horrocks Institute for Mathematics, Physics and Astronomy, University of Central Lancashire, Preston PR1 2HE, United Kingdom
[3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
[4]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305
[5]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[6]Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706
[7]Thomas Lord Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC 27708

We present several complementary projects integrating computational modeling, machine learning, and advanced experimental methods to investigate and control material structures at the atomic scale. These include using density functional theory (DFT) coupled with scanning tunneling microscopy (STM) simulations to analyze semiconductor surface terminations; employing multimodal machine learning frameworks for interpreting spectroscopic data and identifying local elements and defects; nanoscale manipulation and characterization of strongly correlated materials such as VO_2 via oxygen vacancy dynamics; and generating diverse training datasets through molecular dynamics (MD) simulations for enhanced machine learning applications. Together, these approaches significantly advance our understanding, predictive capabilities, and ability to engineer novel material functionalities.

Strain-localized Excitonic Emissions in Two-dimensional Semiconducting Magnet CrSBr

Kiyoung Jo[1], Zdeněk Sofer[2], Jonathan Brunette[3], and Adina Luican-Mayer[1,3]

[1]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Department of Inorganic Chemistry, University of Chemistry and Technology, 16000 Prague, Czech Republic
[3]Department of Physics, University of Ottawa, Ontario K1N 6N5, Canada

Two-dimensional (2D) materials allow the exploration of previously inaccessible basic physics phenomena in low dimensions. In particular, 2D magnetism has emerged as a promising platform for developing novel magneto-optical, magnetoelectric, and spintronic devices. Among 2D magnetic materials, CrSBr—an anisotropic, air-stable, magnetic semiconductor [1]— has garnered significant attention for its stable exciton, magnetic order bound to its lattices. These intertwined degrees of freedom give rise to rich light-matter interactions including exciton-magnon coupling [2], exciton-lattice interaction [3], and cavity-enhanced polariton [4].

Importantly, such quantum phenomena can be tuned through external control of magnetic order and lattice strain, offering both fundamental insights and practical utility for device applications [5]. However, its excitonic responses—especially those governed by local strain and spin order—remain largely unexplored.

In this work, we investigate excitonic behavior induced by localized strain in CrSBr. Few-layered CrSBr flakes were transferred onto pre-patterned SiO_2/Si substrates containing cylindrical and rectangular trench structures, inducing spatially varying uniaxial or biaxial strain in the range of 0.1–1%. Using optical spectroscopy and scanning probe techniques, we correlate the polarization dependent excitonic responses to both local strain and spin order. Our results reveal that the spin configuration is influenced by strain, which, in turn, affect the excitonic photoluminescence. These findings highlight the potential of strain engineering in controlling spin-exciton interactions in 2D magnetic semiconductors and open new opportunities for quantum transduction at the atomically thin magneto-optoelectronic devices.

Work performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, was supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1] Nano Letters, 2024, 24 4319
[2] Nature Materials, 2025, 24, 391
[3] ACS Nano, 2024, 18, 2898
[4] Nature Communications, 2023, 14, 5966
[5] Nature Nanotechnology, 2022, 17, 3, 256

C-55

Metal Oxide Nanoparticles by Molten Salt Synthesis with High Luminescence Quantum Yield for Salivary Protein Detection

Yuchen Zhang[1] and Yuanbing Mao[1]

[1]Department of Chemistry, Illinois Institute of Technology, Chicago, IL 60616

Highly efficient light-emitting nanoparticles are important for energy conversion and light emission devices along with many potential applications in bio-imaging and bio-labeling areas. The latter applications demand nanoparticulated phosphors with a uniform shape and size, good dispersibility in aqueous media, high chemical stability, and surface-functionalization. These characteristics could be major bottlenecks and hence limit their practical applications. Here I will describe a simple combined coprecipitation-molten salt method to synthesize highly uniform $Zn_2GeO_4:Mn^{2+}$ nanoparticles (NPs) using NaCl-KCl as reaction environment. A thorough characterization of these NPs has shown that the MSS process is essential to realizing uniform NPs as the salt acts as a surface protection agent. We have evaluated the luminescence properties of the $Zn_2GeO_4:Mn^{2+}$ NPs with different doping levels of Mn^{2+} (0.2–2.00mol%) and found the optimum Mn^{2+} doping level for the highest photoluminescence (0.50% Mn) and the longest persistent luminescence to be 0.50%. Surfaced coating with (3-aminopropyl) triethoxysilane and active C-reactive protein antibody as biomarkers has provided high colloidal stability to the $Zn_2GeO_4:Mn^{2+}$ NPs through electrostatic and steric interactions as these surface charging groups act as anchor sites for the conjugation of biomolecules to their surface. These NPs are chemically stable for at least one week in phosphate buffer saline (pH range = 6.0–7.4). Taking advantage of such properties and the presence of surface carboxylate groups, we have used the surface-functionalized $Zn_2GeO_4:0.50\%Mn^{2+}$ NPs to develop a persistent luminescence-based immunoassay for the autofluorescence-free detection of C-reactive protein in PBS buffer solution and artificial saliva. This study demonstrates that our persistently luminescent $Zn_2GeO_4:0.50\%Mn^{2+}$ NPs are ideal candidates for bio-applications in imaging, labeling and protein detection.

C-56

Spectroscopic Analysis of Polymer and Monolayer MoS_2 Interfaces for Photodetection Applications

Christine K. McGinn[1,2], Daniel M. Harrington[2], Edwin Heilweil[2], and Christina A. Hacker[2]

[1]Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago, IL 60607
[2]National Institute of Standards and Technology, Gaithersburg, MD 20899

Two-dimensional transition-metal dichalcogenides (2D TMDs) have been extensively studied for photodetection applications due to their strong optoelectronic behavior in the visible range and tunable band gap [1]. 2D TMD field effect transistors (FETs) have the advantage of large ON/OFF ratio and small form factor compared to other transistor-based photodetectors [2]. However, the optoelectronic properties of 2D TMDs can deteriorate as a result of surface defects and exposure to air and water. Researchers have used a variety of materials to combat this degradation and passivate the surface, most commonly hexagonal boron nitride. Polymers are ideal for passivating 2D TMDs in photodetection applications as most are transparent in the visible range, and improvement in photodetection by polymer encapsulation has been previously shown [3].

Polymer passivation has been leveraged to improve photodetection in two dimensional transition metal dichalcogenide field-effect transistors (2D TMD FETs). The relative passivation effects of common polymers, however, is not well understood. In this work, the interface of monolayer MoS_2 and three common polymers, Parylene N (Pa-N), polymethyl methacrylate (PMMA), and polyvinylidene difluoride trifluoroethylene (PVDF-TrFE), is assessed with multiple spectroscopic methods. Raman and photoluminescence spectroscopy demonstrate that Pa-N and PMMA provide an n doping effect, which increases photoconductivity and photogenerated charge in Terahertz domain and time-resolved spectroscopy. Terahertz time-resolved spectroscopy shows significantly longer carrier lifetime for MoS_2 coated with PVDF-TrFE compared to other polymers. These results suggest that PVDF-TrFE provides a unique benefit for photodetection applications beyond its ferroelectric properties [4].

[1] Nalwa, Hari Singh. *RSC advances* 10, no. 51 (2020): 30529-30602.
[2] Wu et al. *The Journal of Physical Chemistry Letters* 4, no. 15 (2013): 2508-2513.
[3] Ma et al. *Applied Physics Letters* 113, no. 1 (2018).
[4] McGinn, Christine K., et al. *Applied Physics Letters* 124, no. 1 (2024).

A-57

Colloidal Crystal Engineering with DNA

Ana Clara Zampirolli Leal[1,2], Rachel R. Chan[1,2], and Chad A. Mirkin[1,2]

[1]Department of Chemistry, Northwestern University, Evanston, IL 60208
[2]International Institute for Nanotechnology, Northwestern University, Evanston, IL 60208

Over the past two decades, synchrotron x-ray radiation characterization techniques, including small-angle x-ray scattering (SAXS) and x-ray diffraction, have been foundational to the study of DNA-mediated assembly of nanoparticle building blocks to form colloidal crystals. This approach to organizing nanomaterials leverages programmable DNA hybridization events to direct colloidal crystal formation with control over lattice parameter, symmetry, crystal size, and shape. Given that the anisotropy, size, and composition of the nanoparticle core is decoupled from the DNA design, a swath of nanoscale building blocks, spanning from metals to proteins, can be organized into crystalline materials using this approach. Indeed, to date, colloidal crystal engineering with DNA has led to the determination of > 90 lattice symmetries and enabled the design of materials with exotic properties, including high specific strength, shape memory, negative refractive index, and nonlinear optical responses. The high flux and resolution of the Advanced Photon Source have been critical in examining the structures of these materials with nanoscale periodicities. Moving ahead, new capabilities of the upgraded APS (such as x-ray ptychography imaging) will elucidate structural information that was not previously attainable, enabling the design of next-generation colloidal crystals engineered with DNA.

Development of Gold-copper Nanorod-based Catalysts with Controlled Plasmon-mediated Selectivity, Optimized Activity, and Enhanced Stability for CO_2 Reduction

Siyu Zhou[1], Emily Cook[1], and Catherine Murphy[1,2]

[1]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, IL 61801
[2]Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL 61801

This project aims to develop Au@AuCu nanorod catalysts (core: gold (Au); shell: gold–copper (Au–Cu) alloy) for plasmon-driven carbon dioxide (CO_2) reduction, with the goal of maximizing catalytic activity and stability under controllable selectivity. One key focus is to systematically investigate how plasmon wavelength affects product selectivity. As confirmed by transmission electron microscopy (TEM) and ultraviolet–visible spectroscopy (UV–vis), Au–Cu nanorods with tunable aspect ratios can be synthesized to generate localized surface plasmon resonances (LSPRs) over a wide range of wavelengths. Each wavelength corresponds to the energy state of specific reaction intermediates, enabling selective activation toward targeted products such as hydrocarbons [1,2,3]. To probe this relationship, I will use *in-situ* Raman vibrational spectroscopy at Argonne National Laboratory to detect key intermediates under different LSPR conditions, which may help guide existing reaction pathways or unlock new ones. Building on this selectivity control, I aim to further optimize the activity and stability of Au@AuCu nanorods by tuning the Au–Cu shell thickness and copper composition, as confirmed by TEM and inductively coupled plasma mass spectrometry (ICP-MS). Considering the asymmetric structure of the nanorods, I also employed energy-dispersive x-ray spectroscopy (EDS) tomography and four-dimensional scanning transmission electron microscopy (4D-STEM) to map the elemental and strain distributions across different regions (tips, side facets, and interior), enabling more accurate identification of active sites and structure–activity correlations. For selected nanorods with promising performance, I plan to use synchrotron-based *in-situ* x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectroscopy (XAS) to study their electronic and structural dynamics under reaction conditions. This is essential, as plasmonic excitation may cause issues such as local overheating, copper oxidation, or nanoparticle sintering. These *in-situ* studies will not only help determine which combinations of Cu composition and shell thickness offer the best stability, but also clarify the mechanisms of catalyst deactivation, providing a clear direction for improving durability, which remains a key barrier to the commercialization of plasmon-enhanced catalysis.

[1] Aslam, U.; Rao, V. G.; Chavez, S.; Linic, S. Catalytic Conversion of Solar to Chemical Energy on Plasmonic Metal Nanostructures. *Nat. Catal.* 2018, *1*, 656–665.
[2] Boerigter, C.; Campana, R.; Morabito, M.; Linic, S. Evidence and Implications of Direct Charge Excitation as the Dominant Mechanism in Plasmon-Mediated Photocatalysis. *Nat. Commun.* 2016, *7*, 10545.
[3] Yu, S.; Wilson, A. J.; Heo, J.; Jain, P. K. Plasmonic Control of Multi-Electron Transfer and C-C Coupling in Visible-Light-Driven CO_2 Reduction on Au Nanoparticles. *Nano Lett.* 2018, *18*, 2189–2194.

OTHER

A-59..Chodankar, Abhijeet

Optimization of LMR-NMC Cathodes Using Genetic Algorithms

Abhijeet D. Chodankar[1], Pallab Barai[1], and Venkat Srinivasan[2]

[1]Applied Materials Division, Argonne National Laboratory, Lemont, IL 60439
[2]ACCESS, Argonne National Laboratory, Lemont, IL 60439

Energy storage devices play a critical role in enhancing national security, improving grid resilience, and supporting advanced computing infrastructures essential for America's technological leadership. Batteries using manganese-rich cathode materials are important for the United States as they diversify the battery supply chain, decrease dependence on limited and geopolitically sensitive resources such as cobalt and nickel, lower battery costs, and enable greater energy storage capacity.

The primary objective of this research is to enhance the energy density of lithium-rich manganese-rich nickel-manganese-cobalt oxide (LMR-NMC) cathode materials. Computational modeling has proven to be an essential tool for experimentalists in optimizing parameters related to electrode design. However, conventional battery models do not adequately account for the microstructure of secondary particles or the electrolyte diffusion pathways within agglomerate pores. The agglomerate model addresses this gap by capturing multiscale lithium diffusion within both electrode pores and primary particles in the agglomerates, allowing accurate estimation of actual battery capacity.

This research aims to maximize the energy density of LMR-NMC cathode materials by employing a genetic algorithm to systematically explore critical parameters that significantly influence electrochemical performance. The results from this research will provide optimized electrode design guidelines, contributing to improved battery performance.

PHYSICS

ESRP: Solving for the Hydrogen Emission Spectrum and Energy Levels

Erhem (McKayla) Bolor[1], Laura Dogium[1], Brandon Dohmeier[1], Dylan Hoag[1], Timothy Kwok[1], Muhammad (Firdaus) Nuriddin[1], Kyra Pierce[1], Phallon Pierce[1], Ishika Rana[1], Gabriel (Lake) Whatcott[1], Lois Emde[1], and Paul Chow[2]

[1]Bolingbrook High School, Bolingbrook, IL 60440
[2]Sector 16-ID-D, Argonne National Laboratory, Lemont, IL 60439

The purpose of the experiment was to understand the relationship between hydrogen atoms and Schrödinger's wave equation, which describes the form of the probability waves that govern the motion of small particles and specifies how these waves are altered by external influences. By comparing experimental results from the hydrogen emission spectrum found using an optical spectrometer with calculations made for the hydrogen atom energy levels and emission spectrum, the quantum relationship's origins can be learned, in addition to the discrete energy levels that make up the foundation of quantum physics.

The team solved Schrödinger's wave equation for the energy levels of the hydrogen atom. Using these findings as a baseline, the team built an optical spectrometer that effectively disperses light from excited hydrogen atoms into its constituent wavelengths via a prism or diffraction grating, allowing the observation of a spectrum of distinct colored lines on a screen that corresponds to specific transitions between electronic orbital energy levels within the hydrogen atom.

Schrödinger's wave equation enables the mathematical finding of the position of a hydrogen atom's electrons in its orbitals. Since it describes the behavior of waves, the wave equation contributes to further advances in understanding other phenomena such as light waves and sound waves. Being able to utilize Schrödinger's wave equation enhances the study of atomic structures and wave behaviors which has a prominent impact in understanding why atoms emit light at certain wavelengths when excited. Schrödinger's wave equation largely helps the understanding of light waves. This has a profound impact as certain wavelengths of light can be used in the medical field to sterilize equipment and visible light waves are utilized in various medical devices to allow physicians to see inside patients.

ESRP: Quantum Mechanics and Spectroscopy

Adrian Cruz[1], Amira White[1], Asmaa Shaibat[1], Ayoub Alwahsh[1], Carter Rohe[1], Leilani Avila[1], Steven Cozen[1], Valente Ornelas Jr.[1], Sheri Caine[1], and Paul Chow[2]

[1]Harold L. Richards High School, Oak Lawn, IL 60453
[2]HPCAT Sector 16-ID-D, Argonne National Laboratory, Lemont, IL 60439

The Richards High School ESRP team used a spectroscope to analyze the emission spectrum of hydrogen to understand how this data supports Schrödinger’s equation and the concept of wave functions. Schrödinger’s equation is a fundamental equation in quantum mechanics that describes how the wave function changes over time. The wave function itself describes how matter is a probability wave similar to light waves. When squaring the absolute value of the wave function, one can find the probability of locating an electron at a particular position.

The first several months of this project were dedicated to understanding the calculus required to solve Schrödinger’s equation for hydrogen. Once the ESRP team had a solid understanding of the mathematics, the focus shifted to the relationship between the probability of finding an electron a certain distance from the nucleus and the emission spectra of hydrogen (addressing the Lyman, Balmer, and Paschen series). While the energies of the hydrogen atom can be described by the quantum number n, the team discussed how the wave function requires three quantum numbers to represent the three dimensions in which the electron can move.

Finally, using a hydrogen gas discharge tube, power supply box, and PASCO spectroscope, the team measured and recorded the wavelengths of the spectral lines observed in the hydrogen spectrum at Richards High School in Oak Lawn using materials funded by Community High School District 218. By plotting the recorded wavelengths on graph paper, the team compared the observed wavelengths to the known values from the hydrogen spectrum. Through the lessons in the calculus needed for quantum mechanics, the team related the energy levels of the electron in hydrogen to the wave function of the hydrogen atom in Schrödinger’s equation. Finally, the team discussed the error between the calculated and experimental values.

Understanding Schrödinger’s equation and the mathematics involved is crucial for understanding quantum mechanics.

ESRP: Assembly and Characterization of a “Plug-and-Play” Position-sensitive Silicon Detector Array for Use in a Solenoidal Spectrometer (SOLARIS) at the Facility for Rare Isotope Beams (FRIB) at Michigan State University

Jacob Bobek[1], Michael Dierkes[1], Bridget Ferriter[1], Javier Gonzalez[1], Elizabeth Henderson[1], Emilie Knaack[1], David Krzysiak[1], Natalie Krumdick[1], Xochitl Sekiya[1], William Kane[1], Benjamin Kay[2], and Russell Knaack[2]

[1]Lockport Township High School, Lockport, IL 60441
[2]Physics Division, Argonne National Laboratory, Lemont, IL 60439

In the late 2000s, Argonne National Laboratory pioneered a new technology for studying nuclear reactions with radioactive ion beams called single-nucleon transfer reactions, where individual protons or neutrons are added to the beam [1]. In this regime, the reactions are said to be carried out in inverse kinematics (heavier beam impinges upon a light target) as opposed to traditional approaches with stable ion beams (light beam impinges a heavy target). The challenge introduced in inverse kinematics is a so-called “kinematic compression,” which results in a loss of resolving power (peaks in a spectrum move closer together and overlap). The concept to overcome this kinematic compression was realized in the form of the HELIcal Orbit Spectrometer (HELIOS) [2]. Using a large solenoidal field (like an MRI magnet of around 3 Tesla) as the scattering chamber for single-nucleon transfer reactions results in the outgoing ions from a reaction tracing out helical orbits along the solenoid axis. Their energy and position can be determined via position-sensitive silicon detectors along the axis of the solenoid. The technique has proven highly successful for nuclear spectroscopy, and similar devices have been developed at CERN’s ISOLDE facility [3] and, recently, the SOLARIS spectrometer at FRIB [4], which is still under development (early science results from this were enabled by a loaned detector system from the HELIOS spectrometer).

For the SOLARIS, two new modular (plug-and-play) position-sensitive silicon detector arrays are under development at Argonne. New silicon detectors arrived at Argonne starting November through January 2025. Essential to the completion of the detector system is the assembly and characterization of the SOLARIS silicon-detector arrays. The arrays are being assembled using 50×10-mm sized position-sensitive sensors, of which a six-sided structure, 10-detectors long will be assembled. The sensors need to be epoxied to “detector” printed circuit boards using custom 3D-printed jugs, then wire bonded. The individual sensors on the “detector” board will then engage with a “master” printed-circuit board. Prior to this each sensor will be characterized, exploring the “IV curve” (the leakage current as a function of voltage) and their intrinsic resolution determined with an alpha source. The assembly and characterization are essential tasks prior to the installation of the silicon-array into the SOLARIS spectrometer. In terms of the SOLARIS project, the timeframe for this project is November 2024 through March 2025.

[1] A. H. Wuosmaa et al., Nucl. Instrum. Methods Phys. Res. A 580, 1290 (2007).
[2] J. C. Lighthall et al., Nucl. Instrum. Methods Phys. Res. A 622, 97 (2010).
[3] The ISOLDE Solenoidal Spectrometer website. https://isolde-solenoidal-spectrometer.web.cern.ch/
[4] The SOLARIS website. https://www.anl.gov/phy/solaris

ESRP-64

ESRP: Investigating the Effects of Ag111 Surface Texture on the Hydrogenation of CO_2

Nozomi Shirato[1], Rachel Cecil[2], Nisitha Gadhi[2], Yunus Khan[2], Prakul Madaan[2], Anushka Menon[2], Omer Mescioglu[2], Sakina Rizvi[2], Serena Sabzaali[2], and Lillian Wallin[2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]Plainfield North High School, Plainfield, IL 60585

The accumulation of atmospheric carbon dioxide is currently at the center of the global climate crisis. To tackle this crisis, we need to investigate methods to increase the efficiency with which we are able to capture/convert atmospheric CO_2. This project will investigate the effects surface texture has on a Ag111 crystal's ability to facilitate the hydrogenation of atmospheric CO_2 ($CO_2 + H_2 \rightarrow H_2O + CO$). Our aim is to show that by increasing the roughness of the crystal's surface we will increase the surface area the target reaction has to take place on, thereby increasing the overall efficiency of using Ag111 for carbon capture/conversion. To characterize the surfaces at atomic resolution a low-temperature scanning tunneling microscope (LT-STM) is utilized. Then, the performance of CO_2 hydrogenation of the nanomaterial is evaluated by temperature-programmed desorption (TPD) measurements. Preliminary data from this experiment shows promise that increasing the surface area on Ag111 crystals does in fact lead to increased rates of the targeted reaction. Results from this investigation open the door to lines of research that will further the development of more efficient atmospheric carbon capture devices in the future.

POLYMERS

Design and Optimization of Conjugated Polymers (CPs) for High-performance Electronics: Chain Conformation with Dimensional Tuning

Sein Chung[1,2], Young Yong Kim[2], and Kilwon Cho[1]

[1]Department of Chemical Engineering, POSTECH, Pohang, 37673 Republic of Korea
[2]Beamline Division, Pohang Accelerator Laboratory, Pohang, 376373 Republic of Korea

Conjugated polymers (CPs) have emerged as promising candidates for future electronics due to their mechanical softness and chemical tunability. CPs demonstrate innovative potential in various applications, including stretchable thin-film transistors (TFTs), solar cells, synaptic transistors, and thermoelectric devices. Establishing structure-performance relationships between the nanostructure of these materials and the performance of electronic devices is crucial for device optimization and performance enhancement. In this context, synchrotron-based nanostructure analysis has proven indispensable, enabling researchers to "visualize the invisible" and elucidate the underlying mechanisms governing device performance.

This presentation will showcase the research focusing on the nanostructure and energetic structure analyses of CPs facilitated by the Pohang Accelerator Laboratory [1-10]. Specifically, findings from various scattering techniques (e.g., (GI/Tr)-mode (S/W) AXS) and photoelectron spectroscopic methods (e.g., XPS, NEXAFS) have revealed critical insights into ordered crystalline structure, conjugated backbone orientation, and energy level conjugated polymers in diverse electronic devices. These advanced characterization techniques have been essential in unraveling the complex structure-performance relationships in CP-based electronics. Furthermore, this research aims to foster potential collaborations and future joint research opportunities with the Advanced Photon Source at Argonne National Laboratory, promoting the continued advancement.

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Science and ICT (MSIT) of Korea and Young Scientist Support Program from Korean Synchrotron Radiation User's Association (KOSUA). Also, the authors thank the Pohang Accelerator Laboratory (PLS-II) for providing the synchrotron radiation source at 3C SAXS-I, 4D PES, 9A U-SAXS, 10A2 HR-PES II beamlines used in this study.

[1] *Adv. Electron. Mater.*, 2021, 7, 11, 2100551
[2] *ACS Appl. Mater. Interfaces.*, 2022, 14, 12, 14588
[3] *Chem*, 2022, 8, 11, 3130
[4] *Adv. Funct. Mater.*, 2023, 33, 23, 2212127
[5] *Sol. RRL*, 2023, 7, 12, 2300267
[6] *Adv. Sci.*, 2023, 10, 26, 2303150
[7] *Adv. Funct. Mater.*, 2023, 33, 50, 2307355
[8] *Chem. Mater.*, 2024, 36, 1, 74
[9] *Adv. Sci.*, 2024, 11, 16, 2400304
[10] *eScience*, 2025, 5, 1, 100305

Material and Mechanical Characterization of SLA 3D-printed Graphene Nanoplatelet-based Nanocomposites Fabricated within a Magnetic Field

Soka Suliman[1], Alisha Diggs[2], and John Shelton[1]

[1]Department of Mechanical Engineering, Northern Illinois University, DeKalb, IL 60115
[2]Department of Biomedical Engineering, Northern Illinois University, DeKalb, IL 60115

The process of utilizing a static magnetic field to fabricate a nanomaterial-based composite via a stereolithography (SLA) 3D printing process is still a relatively new approach within the field of additive manufacturing. By using this magnetic field during the 3D printing process, both material and mechanical properties can be oriented and axially varied for enhanced characteristics. In this investigation, between 0% to 2% volume fractions of high aspect ratio, graphene nanoplatelets (GNP) are suspended within UV-curable resin during a SLA 3D printing process with a static magnetic field applied. The objective of this investigation is to determine the effect of graphene nanoplatelet inclusions on the material and mechanical properties of this nanomaterial-based composite fabricated using the SLA process. The material properties of the nanoparticle, UV-curable resin, and their interface are characterized using scanning electron microscopy, x-ray diffraction spectroscopy, and Raman spectroscopy. The mechanical property that is investigated is hardness.

This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility through the User Proposal 83614, and was supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

TECHNIQUE

Machine Learning Model for Improved Spatial Resolution and Peak Detection in High-energy Diffraction Microscopy

Dishant Beniwal[1], Hemant Sharma[1], Jun-Sang Park[1], Peter Kenesei[1], and Antonino Miceli[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

Far-field High-energy Diffraction Microscopy (FF-HEDM) uses synchrotron radiation for *in-situ* study of 3D grain characteristics in bulk polycrystalline materials and can provide unparalleled insights into the deformation and damage mechanisms [1]. FF-HEDM reconstruction involves mapping of measured diffraction spots to respective grain positions and orientations, and thus the quality of reconstruction is directly dependent on both the spatial accuracy of measured spot locations as well as the ability to deconvolute overlapping peaks. Since subpixel accuracy of peak center detection is needed for strain analysis, this becomes a challenge when using pixel-array detectors where the spatial spread of intensity over the pixel is lost and only the integrated intensity at a pixel is preserved. In this work, we present a machine learning (ML) model (based on convolutional neural networks) that can predict the peak positions as well as detect overlapping peaks with further improved accuracy than the usual analytical peak fitting methods, which may fail to identify peaks or introduce large errors in peak positions at the reconstruction input. The ML model is integrated with the MIDAS workflow for FF-HEDM grain reconstruction. We show that the ML model can reduce the errors in peak positions by up to 10 times and can enable detection of overlapping peaks to isolate grains that have a low misorientation and are located close to each other.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility at Argonne National Laboratory and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. This work was also supported by the DOE Office of Science, Office of Basic Energy Sciences Data, Artificial Intelligence and Machine Learning at DOE Scientific User Facilities program under award No. 08735 (`Actionable Information from Sensor to Data Center').

[1] Bernier, J. V., Suter, R. M., Rollett, A. D. & Almer, J. D. High-Energy X-Ray Diffraction Microscopy in Materials Science. *Annu. Rev. Mater. Res.* 50, 395–436 (2020).

XModFit: X-ray Modeling and Fitting

Mrinal Bera[1]

[1]NSF's ChemMatCARS, Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637

XModFit, a graphical interface tool developed at NSF's ChemMatCARS, enables users to model and fit 1D data. It can model various experimental 1D data types, but its primary focus is on analyzing x-ray scattering data from Liquid Interface X-ray Scattering (LIXS) and Anomalous Small- and Wide-angle X-ray Scattering (ASWAXS) experiments conducted at NSF's ChemMatCARS, Sector 15 of the Advanced Photon Source. XModFit can read and process multicolumn ASCII data as required for analysis by specific models. In addition to the models developed for ChemMatCARS, it provides user-friendly templates for developing new models or modifying existing ones to create new ones. One of XModFit's unique features is its ability to export user-defined parameters generated during model evaluation. It also estimates the uncertainties in fitting parameters and user-defined functions using Markov Chain Monte Carlo methods. Furthermore, XModFit includes calculators that provide energy-dependent x-ray scattering factors for elements and compounds with known stoichiometry, which are essential for LIXS and ASWAXS analysis.

NSF's ChemMatCARS, Sector 15 at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) is supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1834750 and NSF/CHE-2335833. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

[1] Mrinal K. Bera, Wei Bu, XModFit: X-ray Modeling and Fitting, URL: https://github.com/chemmatcars/XModFit/tree/main

Nuclear Resonant Scattering Studies at APS IXN Group

Michael Y. Hu[1], Thomas S. Toellner[1], Barbara Lavina[1], E. Ercan Alp[1], and Jiyong Zhao[1]

[1]X-ray Science Division, Advance Photon Source, Argonne National Laboratory, Lemont,
IL 60439

Sector 3 (3-ID) at the Advanced Photon Source (APS) at Argonne National Laboratory is a high energy-resolution spectroscopy beamline, which develops and applies nuclear resonant scattering (NRS) methods to study architype and functional materials, e.g., magnetic materials, piezo-electric and thermoelectric materials, superconductors, biomimetic materials such as porphyrins, as well as proteins and enzymes, metal-organic frameworks, materials that are of interest to the catalytic cycle, energy storage and transmission, minerals, and synthetic analogs relevant to Earth and planetary sciences.

The nuclear resonant inelastic x-ray scattering (NRIXS) method focuses on determining vibrational dynamics and elastic properties and can infer many thermodynamics properties of materials. Synchrotron Mössbauer spectroscopies (SMS) in either time or energy domain are used to reveal information about valence, ligand symmetry, and magnetism.

Part of the NRS program is carried out at Sector 30 (30-ID). NRS measurements using five isotopes (Kr-83, Fe-57, Eu-151, Dy-161, and Sn-119) are conducted at 3-ID and 30-ID.

Efficient high-energy resolution monochromator and x-ray optics development is of the utmost importance to these types of spectroscopies. Our research activities also include development of novel instrumentations in new application areas, providing extreme conditions of temperature and pressure, and micro-focusing strategies, to cover both spectroscopy and microscopy. A novel energy-domain Mössbauer spectrometer is being developed to enhance NRS capabilities post upgrade.

The upgraded APS delivers various enhancements to nuclear resonant scattering (NRS) programs, including significant improvement of micro focusing capability, much cleaner bunch purity, and better beam quality and stability, enabling better characterization and studies of materials.

As one of the earliest beamlines to be commissioned, 3-ID observed x-ray beam in July 2024 and started technical commissioning. Users were involved in early August 2024 during the scientific commissioning. 30-ID started commissioning in September. General user programs (GUP) at both 3-ID and 30-ID resumed in the fall of 2024.

A-70

Advanced Spectroscopies at S-25

Shelly Kelly[1], Yanna Chen[1], Zou Finfrock[1], Anthony Gironda[1], Juanjuan Huang[1], Debora Motta Meira[1], Rishabh Ranjan[1], Aleks Solovyev[1], George Sterbinsky[1], Chengjun Sun[1], Jiaqi Wang[1], Kamila Wiaderek[1], and Mark Wolfman[1]

[1]Argonne National Laboratory, Lemont, IL 60439

Advanced spectroscopies are in science commissioning at the new APS-U beamline S-25. The new beamline will make use of the APS upgrade with brighter beams with less divergence to collect more x-rays with our 100mm and 300mm KB mirror systems for advanced spectroscopy and imaging. In addition to x-ray absorption measurements of dilute systems, the spectroscopy group has commissioned two new spectrometers – one for high energy resolution fluorescence detection (HERFD) and a second for a new x-ray Raman scattering microscope, which will allow measurements of low energy edges such as C/O/N with 10 KeV x-rays for *in-situ* and *operando* studies. In addition to the new spectrometers for advanced spectroscopies, the spectroscopy group is pioneering the way with the development of Bluesky/Orphyd controls integrated with EPICS to pave the way for automation with user friendly interface. These advances will be discussed.

Enhanced Cryogenic Cooling for Imaging of Large Samples by X-ray Microscopy

Charles Wood[1], Atousa Moayedi[1], Thomas Renshaw[2], Maria Kokkinidou[2], Jonathan Shaxted[2], Lucjan Pajdzik[2], Alex Renshaw[1], and Adriana L. Klyszejko[2]

[1]The Future Technology Centre, University of Portsmouth, Portsmouth PO1 3HE, United Kingdom
[2]Oxford Cryosystems Ltd, Long Hanborough OX29 8LH, United Kingdom

Developments in instrumentation including cryogenic sample environments provide platforms for multimodal tomography application. To increase cryogenic cooling capabilities for large samples, we developed Cryostream 1000 Wide Nozzle. It provides a much larger gas volume when compared to the Standard model and facilitates vitrification of samples up to 3 mm in diameter. The Wide Nozzle has been successfully used to cool large crystals and biological specimens for x-ray and neutron diffraction and scattering studies and hard x-ray microscopy tomography.

We present the development of a lab-based cryogenic hard x-ray imaging system (microCT), designed for sub-micron resolution of biological specimens with reduced need for contrast agents which might affect biological systems.

Utilising the Oxford Cryosystems Cryostream 1000 Wide Nozzle, in conjunction with a Zeiss Versa 610 X-ray Microscope, we demonstrate that delicate biological samples, otherwise degraded under lab x-ray imaging conditions, can be successfully imaged under stable cryogenic conditions over a period of several hours.

Whilst further tests are required, we observed enhancement of absorption contrast and signal-to-noise ratio by reduction of thermal scattering. We visualized fine structural details without heavy metal staining and other associated artefacts that often arise in conventional x-ray imaging.

To map thermal gradients within the cryogenic stream, we used a thermal diode providing precise temperature data across the gas column, helping to guide future optimisation of cooling dynamics. These insights are important for ongoing work aimed at expanding the Cryostream's application to a range of materials, with potential implications for fields like biomedicine, tissue preservation, tomography, aerospace, energy materials, and heritage artefacts.

This cryogenic x-ray system, therefore, represents a significant step towards lab-based cryogenic x-ray imaging, and further developments will focus on quantifying the contributions of x-ray absorption and scatter components at cryogenic temperatures, broadening the system's capabilities for multi-modal microscopy and *in-situ* analyses.

Enhancing Depth Resolution in Multi-slice X-ray Ptychography Using Advanced Reconstruction Techniques

A. Luktuke[1], Y. Jiang[1], J. Deng[1], B. Lai[1], and V. Rose[1]

[1]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

In recent years, x-ray ptychography has emerged as a crucial imaging technique to unveil the intricate structures of materials offering unprecedented resolution. With the Advanced Photon Source upgrade, feature beamlines such as the PtychoProbe will greatly benefit from the increased brightness and be capable of imaging large specimens at sub-10 nm resolution. The reconstruction of such datasets requires an approach that takes wavefield propagation effects into account. Multi-slice ptychography stands out as a significant advancement as it overcomes the inherent limitations of the conventional single-slice model by accommodating the complex scattering effects within thick objects. However, experimental data often lacks sufficient information that guarantees an exact recovery of the 3D structure, resulting in artifacts such as feature blurring, crosstalk, or even random noise. In this study, we delve into several novel approaches to improve the depth resolution of multi-slice ptychography. We investigate sparse angle ptychographic tomography to improve depth resolution, focusing on how to effectively utilize the resulting 3D tomogram. We also assess the impact of advanced reconstruction methods, such as virtual depth sectioning, on the final reconstruction quality. Moreover, we examine deep learning techniques that attempt to mitigate crosstalk artifacts between the reconstructed slices. The systematic evaluation of such novel reconstruction strategies on the simulated and experimental datasets will be discussed in detail.

This work was performed at the Advanced Photon Source, a U.S. Department of Energy Office of Science User Facility under Contract No. DE-AC02-06CH11357.

A-73

Autonomous Reduction and Analysis of 2D Diffraction and Scattering Data

Anna Henckel Merritt[1], Wenqian Xu[1], Olaf Borkiewicz[1], Miaoqi Chu[1], Nicholas Schwarz[1], Brian Toby[1], and James Weng[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

Current analysis methods for powder diffraction and total scattering experiments involve looking at only the 1D integrations of 2D image data. This form of data reduction does not retain information such as preferred orientation or location and number of single crystal diffraction spots.

The primary goal of this project is to develop a data analysis and reduction pipeline which retains such information while autonomously performing common steps such as masking and integration for the user. These results are then shown to the user in a convenient user interface in real time. The first step in retaining the 2D information is classification of outlier pixel clusters into spots and texture arcs. The differences in integrating with and without each set of outliers is shown to the user in a UI alongside the original image and outlier masks to aid in identifying peaks resulting from each type. Statistics on the position and area of these clusters as well as the cosine similarity between subsequent images are also shown in the UI.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility and is based on work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. DOE under Contract No. DE-AC02-06CH11357. (Proposal 2024-0044)

Precise Position Control of Sample Region of Interest within the Scattering Volume

Carol Thompson[1] and G. Brian Stephenson[2]

[1]Department of Physics, Northern Illinois University Dekalb, IL 60115
[2]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439

A sample region of interest (ROI) wandering away from the initial beam-sample intersection point during angle and hkl-scans is a well-known occurrence. The motions are amplified with various common diffractometer-beamline-sample misalignments. For many scattering studies, relative scattering volume motions are within the requirements of the experiment and alignment protocols can minimize the wandering. However, as typical beam sizes become small with the APS upgrade, there is a need for more precise control of the illumination on a small ROI under different scattering conditions with wide variation of angles (e.g., collecting multiple reciprocal space maps at different Bragg Peaks during BCDI experiments or diffraction on microfeatures.)

We describe a straightforward methodology to calculate the translations required to keep a fixed region illuminated during scans or after large angular reconfigurations. Our initial motivation was to understand these effects and their implications for operation of the CHEX beamline hexapod diffractometer design that combines sample positioning with angular motion. However, the methodology is easily generalized to any diffractometer design. The algorithms are based on a 4×4 matrix operator formalism defining rotation and translation operators. They can be used to keep the same point on the sample in the incident beam during scans, even if it is not on the center of rotation (COR). They correctly account for beam-sample wandering that occurs during scans or large multiple angular excursions as a function of various misalignment issues such as 1) transverse offsets of incident beam trajectory from the COR, 2) upstream-downstream offsets of beam-sample scattering region from the COR, and 3) mechanical misalignment errors or translations of rotation axes (when rotation axes do not intersect at conventionally defined COR).

Supported by US Department of Energy (DOE), Office of Science, Office of Basic Energy Science, Materials Sciences and Engineering Division.

A Survey of Image Registration Methods for Multi-scale, Multi-modal Imaging Data Analysis

Xiaozhi Zhang[1], Zichao Di[1,2], Josh Han[1], Yanqi Luo[1], Robin Pourzal[3], and Si Chen[1]

[1]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[2]Mathematics and Computer Science, Argonne National Laboratory, Lemont, IL 60439
[3]Department of Orthopedic Surgery, Rush University Medical Center, Chicago, IL 60612

Imaging of biological samples, including tissue sections, organoids, and cells, provides critical insights into their structure, function, and pathology. Multi-scale, multi-modal imaging enhances these insights by integrating data from various imaging and analytical techniques, providing a more comprehensive understanding of complex biological systems.

To fully leverage the richness of these diverse datasets, accurate image registration is essential. Aligning images acquired at different scales and resolutions into a common coordinate system maximizes the interpretability and utility of the data.

Herein, we present a comparative survey of several image registration methods and evaluate their performance using both simulated and experimental datasets. Our initial efforts focus on multi-scale images obtained using synchrotron-based x-ray fluorescence (sXRF) microscopy, which will be extended to include results from optical and electron microscopy. We aim to propose a practical workflow for multi-scale, multi-modal image integration to facilitate robust data analysis and advance research applications.