MAY 2019

Argonne NATIONAL LABORATORY

2019 APS/CNM USERS MEETING

Program and Abstracts

2019 APS/CNM USERS MEETING

PROGRAM AND ABSTRACTS

User Facilities at Argonne National Laboratory

User Contacts

Advanced Photon Source
http://www.aps.anl.gov
630-252-9090
apsuser@aps.anl.gov

Argonne Leadership Computing Facility
http://www.alcf.anl.gov
630-252-0929

Argonne Tandem Linac Accelerator System
http://www.phy.anl.gov/atlas
630-252-4044

Center for Nanoscale Materials
http://nano.anl.gov
630-252-6952
cnm_useroffice@anl.gov

Table of Contents

The 2019 APS/CNM Users Meeting theme recognizes 2019 as the International Year of the Periodic Table of Chemical Elements.

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About Argonne National Laboratory

Argonne is a U.S. Department of Energy laboratory managed by the UChicago Argonne, LLC under Contract No. DE-AC02-06CH11357. The Laboratory is located southwest of Chicago at 9700 South Cass Avenue, Lemont, Illinois 60439. For information about Argonne, see www.anl.gov.

2019 APSUO Compton Award
Prof. Tai-Chang Chiang
(University of Illinois at Urbana-Champaign)

Professor Tai-Chang Chiang, Emeritus and Research Professor of Physics at the University of Illinois at Urbana-Champaign (UIUC), has been chosen to receive the 2019 Arthur H. Compton Award, presented by the Advanced Photon Source Users Organization (APSUO), "for his ingenuity and insight in developing x-ray thermal diffuse scattering into an efficient quantitative method for phonon band structure studies."

Beginning in the 1980s, Prof. Chiang was a pioneer in the use of synchrotron radiation in establishing the angle-resolved photoemission technique for electron band structure determination of solids, surfaces, and films.

His more recent scientific accomplishment is in developing the thermal diffuse scattering (TDS) technique into an efficient, quantitative method by which materials scientists at synchrotron x-ray facilities such as the Advanced Photon Source (APS) can determine phonon band structure. The impact of this methodology on materials research, especially in cases involving small samples, microstructures, and phase transitions is likely to be far reaching.

The TDS scattering patterns, recorded with a two-dimensional detector, show intricate details involving phonons from a wide range in k space over many zones. For instance, a least-squares analysis of the data acquired in just 20 seconds at APS Sector 33 yielded phonon dispersion curves of silicon over the entire Brillouin zone, which are in excellent agreement with neutron scattering results. This work was cited by Prof. Millie Dresselhaus in a plenary talk at the 2000 Fall MRS Meeting as one of three major achievements from all U.S. Department of Energy (DOE) facilities. The results were adopted by Jens Als-Nielsen and Des McMorrow in their textbook, *Elements of Modern X-Ray Physics* (Wiley, 2001), pg. 141.

Chiang's group has since extended the work to a variety of systems and phenomena. Particularly notable research includes phonon softening in the charge-density-wave compound TiSe2; phonon anomalies in niobium and plutonium; renormalization and fluctuation effects associated with the antiferrodistortive transition in $SrTiO_3$; and a new method of direct data inversion based on momentum-resolved x-ray calorimetry.
Ian K. Robinson
Professor of Physics, University College London

Over the course of his career, Prof. Chiang has made lasting contributions to condensed matter physics, surface science, and synchrotron radiation research, including several truly groundbreaking findings. He has authored some 300 journal articles, and his work has been cited more than 8500 times.

Chiang's work on precision electron spectroscopy and structural determination has led to important advances in the physics of electrons, lattice structures, and phonons and their mutual interactions in solids, at surfaces, in films, and at the nanoscale.

In 2016, he was elected by the Academia Sinica to its 2016 class of Academicians. He was among 22 scholars across all academic disciplines to receive that high honor that year. Academia Sinica is the national academy of Taiwan.

Chiang is the recipient of numerous other recognitions, including the 2015 Davisson-Germer Prize in Atomic or Surface Physics, sponsored by the American Physical Society. He received the Xerox Award for Faculty Research (1985), the National Science Foundation Presidential Young Investigator Award (1984-89), and the IBM Faculty Development Award (1984-5). He is a Fellow of the American Physical Society.

He served as head of the UIUC Solid State Sciences and Materials Chemistry Program from 1991 to 2006. He was associate director of the Frederick Seitz Materials Research Laboratory at UIUC from 1999 to 2006. From 2003 to 2008, he chaired the Board of Governors for the University-National Laboratory-Industry Collaborative Access Team at the Advanced Photon Source. From 2010 to 2014, he served as the scientific director of the University of Wisconsin-Madison Synchrotron Radiation Center. He was appointed Chair Professor at the National Chiao-Tung University at Taiwan (2013-16); Honorary Chair at National Tsing Hua University at Taiwan (2008-11); and Distinguished Chair at National Taiwan University (2007-10 and 2015-present). He is currently a visiting professor at Tokyo University.

Prof. Chiang received a bachelor's degree in physics from the National Taiwan University in 1971 and a doctoral degree in physics from the University of California, Berkeley, in 1978. He held a postdoctoral appointment at the IBM T.J. Watson Research Center in Yorktown Heights from 1978 to 1980, before he joined the faculty in the Department of Physics at the University of Illinois Urbana-Champaign in 1980.

About the Award

The Arthur H. Compton award was established in 1995 by the APS Users Organization to recognize an important scientific or technical accomplishment at the Advanced Photon Source. The award consists of a plaque and $2500.

The bi-annual awards are presented at the APS/CNM User Meetings, which are held every spring. A call for nominations is sent out before the meeting, and the winner(s) is invited to give an award lecture at the meeting. Awards are not necessarily made each year.

Compton was an American physicist who won the Nobel Prize for Physics in 1927 for discovering and explaining changes in x-ray wavelengths resulting from x-ray collisions with electrons, the so-called Compton effect. This important discovery in 1922 confirmed the dual nature (wave and particle) of electromagnetic radiation. A Ph.D. from Princeton University, Compton held many prominent positions, including professor of physics at The University of Chicago and chairman of the committee of the National Academy of Sciences that studied the military potential of atomic energy. His position on that committee made Compton instrumental in initiating the Manhattan Project, which created the first atomic bomb.

The Advanced Photon Source is a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Argonne National Laboratory seeks solutions to pressing national problems in science and technology. The nation's first national laboratory, Argonne conducts leading-edge basic and applied scientific research in virtually every scientific discipline. Argonne researchers work closely with researchers from hundreds of companies, universities, and federal, state and municipal agencies to help them solve their specific problems, advance America's scientific leadership and prepare the nation for a better future. With employees from more than 60 nations, Argonne is managed by UChicago Argonne, LLC, for the U.S. DOE Office of Science.

The U.S. Department of Energy's Office of Science is the single largest supporter of basic research in the physical sciences in the United States and is working to address some of the most pressing challenges of our time. For more information, visit the **Office of Science website**.

Previous award recipients

Nikolai Vinokurov and Klaus Halbach (1995)

Philip M. Platzman and Peter Eisenberger (1997)

Donald H. Bilderback, Andreas K. Freund, Gordon S. Knapp, and Dennis M. Mills (1998)

Sunil K. Sinha (2000)

Wayne A. Hendrickson (2001)

Martin Blume, L. Doon Gibbs, Denis McWhan, and Kazumichi Namikawa (2003)

Günter Schmahl and Janos Kirz (2005)

Andrzej Joachimiak and Gerold Rosenbaum (2007)

Gerhard Grübel, Simon Mochrie, and Mark Sutton (2009)

Edward Stern, Farrel Lytle, Dale Sayers (posthumously), and John Rehr (2011)

David E. Moncton, John N. Galayda, Michael Borland, and Louis Emery (2013)

Gene E. Ice, Bennett C. Larson, and Cullie J. Sparks (2015)

COMPREHENSIVE PROGRAM

Monday, May 6

8:00 – 5:00 Exhibits
Building 402, Gallery (lower level), outside E1100/1200 and Building 402, Atrium

7:30 – 5:00 Registration
Building 402, Atrium

12:00 – 1:30 Lunch (in the Tent)

Opening Session—Morning
Building 402, Lecture Hall

Session Chairs **R. Joseph Kline, R. Joseph Kline, Leader of Dimensional Metrology for Nanofabrication Project, National Institute of Standards and Technology and Olga Makarova, Creatv MicroTech, Inc.**

8:30 – 8:35 R. Joseph Kline, Chair, APS Users Organization
and Olga Makarova, CNM Users Executive Committee
Welcome and Launch of the 2019 Meeting

8:35 – 8:45 Paul K. Kearns, Argonne Laboratory Director
Welcome from the Laboratory

8:45 – 9:10 Bruce Garrett, Director of the Chemical Sciences, Geosciences, and Biosciences Division, Basic Energy Sciences, DOE
The DOE Perspective

9:10 – 9:25 Dennis Mills, Member of the Board of Directors for the Society for Science at User Research Facilities (SSURF)
Update on the Society for Science at User Research Facilities

9:25 – 9:30 Stephen Streiffer, APS Director
Introduction of Keynote Speaker

9:30 – 10:10 Keynote: Dan Nocera (Harvard University)
APS Insights to Metal-Oxygen and Metal-Halide Bond Activation for Energy Storage

10:10 – 10:35 Break

10:35 – 10:50 Stephen Streiffer, APS Director
APS Update

10:50 – 11:05 Supratik Guha, CNM Director
CNM Update

11:05 – 11:20 Robert O. Hettel, APS Upgrade Director
APS Upgrade Update

11:20 – 11:25 R. Joseph Kline, Chair, APS Users Organization
and Olga Makarova, CNM Users Executive Committee
Introduction of the Speed Science Slam

11:25 – 11:45 S^3: Speed Science Slam
APS: Roman Ezhov (Purdue University)
New Pathways in Iron-based Water Oxidation Catalysis

CNM: Tejas Guruswamy (Argonne National Laboratory)
Hard X-ray Transition Edge Sensors at the Advanced Photon Source

APS: Prabhat KC (Argonne National Laboratory and The University of Chicago)
Convolutional Neural Network Based Super Resolution for X-ray Imaging

CNM: Dali Sun (North Carolina State University)
Spintronic Terahertz Emission by Ultrafast Spin-charge Current Conversion in Organic-inorganic Hybrid Perovskites/Ferromagnet Heterostructures

11:45 – 12:00 Visit with Exhibitors

12:00 – 1:30 Lunch (in the Tent)

Parallel Facility Plenary Sessions—Afternoon

APS Session
Building 402, Lecture Hall

Session Chair: Carlo Segre, Illinois Institute of Technology

1:30 – 1:50 Oliver Schmidt (Argonne National Laboratory)
The APS Upgrade Beamlines Overview

1:50 – 2:30 2019 Arthur H. Compton Award Presentation and Talk:
Tai-Chang Chiang (University of Illinois, Urbana-Champaign)
X-ray Thermal Diffuse Scattering: History, Advances, and Opportunities

2:30 – 3:10 Yulia Pushkar (Purdue University)
X-ray Imaging and Spectroscopy of the Brain

3:10 – 3:25 Break

3:25 – 3:40 Student Invited Talk: Saugat Kandel (Northwestern University)
On the Use of Automatic Differentiation for Phase Retrieval

3:40 – 4:20 Melissa Sims (Johns Hopkins University)
Simulating Meteor Impacts in the Diamond Anvil Cell

4:20 – 5:00 Lin Chen (Argonne National Laboratory and Northwestern University)
Peeking into Excited State Trajectories with Pulsed X-rays: A Journey of Two Decades

5:00 Adjourn

6:00 Banquet
“Synchro De Mayo”
Argonne Guest House and Patio

Parallel Facility Plenary Sessions—Afternoon

CNM Session
Building 402, Room A1100

Session Chair: James Rondinelli, Northwestern University

1:30 – 2:15 Keynote Speaker: Ali Yazdani (Princeton University)
Visualizing Novel Quantum States of Matter

2:15 – 3:00 Paul Evans (University of Wisconsin at Madison)
Expanding the Scope of Nanobeam Diffraction: Dynamical Diffraction in Epitaxial Electronic Materials

3:00 – 3:20 Break

3:20 – 3:30 James Rondinelli, Chair, CNM Users Executive Committee (Northwestern University)
Update from the CNM Users Executive Committee

3:30 – 4:00 Hui Claire Xiong (Boise State University)
Development and Understanding of the Origin of Irreversibility in Layered Transition-metal Oxide Cathode Material for Sodium Ion Batteries

4:00 – 4:30 Peijun Guo (Argonne National Laboratory)
Hybrid Organic-inorganic Perovskites: From Anisotropic Excitons to Soft Crystal Lattice

4:30 – 4:45 Student Invited Talk: Frank Barrows (Northwestern University)
Fabrication, In Situ *Biasing, Electron Holography, and Elemental Analysis of Patterned and Unpatterned TiO_2 Thin Films*

4:45 Adjourn

6:00 Banquet
"Synchro De Mayo"
Argonne Guest House and Patio

Tuesday, May 7

8:00 – 5:00 Exhibits
Building 402, Gallery (lower level), outside E1100/1200 and Building 402, Atrium

8:00 – 5:00 Registration
Building 402, Atrium

8:30 – 12:00 Facility Specific Workshops

12:00 – 2:00 Poster Setup
(shuttle buses and vans provided throughout the lunch hour to provide transportation between APS, the Guest House, and TCS Building 240)

12:00 – 1:30 Lunch (in the Tent)

1:30 – 5:00 Facility Specific Workshops

5:30 – 8:00 Poster Session
TCS Building 240, Shuttle service available

Parallel Facility-specific Workshops

APS/CNM Workshop 1 – Building 402, Room E1100/1200
Driving Scientific Discovery with Artificial Intelligence, Advanced Data Analysis (see page 25)

APS Workshop 3 – Building 401, A1100
Workshop on Chemical Separations (see page 35)

CNM Workshop 4 – Building 401, Room A5000
Photon Qubit Entanglement and Transduction (see page 42)

APS Workshop 7 – Building 446, Conference Room
In Situ *and Multimodal Microscopy for APS-U (see page 57)*

Wednesday, May 8

8:00 – 1:30 Exhibits
Building 402 Gallery, outside E1100/1200 and Building 402 Atrium

8:00 – 1:30 Registration
Building 402, Atrium

8:30 – 12:00 Facility Specific Workshops

12:00 – 1:30 Lunch (in the Tent)

1:30 – 5:00 Facility Specific Workshops

Parallel Facility-specific Workshops

APS/CNM Workshop 2 – Building 401, Room A1100
Topological Quantum Information Science (see page 30)

APS Workshop 5 – Building 402, Room E1100/1200
RIXS after the APS Upgrade: Science Opportunities (see page 47)
Sponsored by Kohzu

CNM Workshop 6 – Building 446, Conference Room
Optoelectronic Devices and Mechanical Systems Based on Ultra-thin 2D Materials (see page 52)

Thursday, May 9

CNM Short Courses

8:30 – 12:00 CNM Short Course A: Building 440, Room B108 (attendees should meet in the CNM Lobby)
Introduction to Confocal Raman Spectroscopy
Instructor: Dave Gosztola (CNM)

A hands-on demonstration of the capabilities of the CNM's confocal Raman microscopes will be presented. Subjects to be discussed and demonstrated include the following:

- Basic Raman spectroscopy concepts
- Anatomy of a confocal Raman microscope
- Sample preparation
- Simple spectra collection
- Effects of excitation wavelength
- Point mapping
- Line/area mapping
- Heating and cooling samples

1:00 – 4:30 CNM Short Course B: Building 440, Room A105/106
Use of Machine Learning in Nanoscale Materials Modeling
Special Requirement: Bring your own laptop
Instructors: Maria Chan and Subramanian Sankaranarayanan (CNM)

This short course will include instructions on the use of machine learning for (1) force field parameterization from first principles data, and (2) nanoscale structure determination from a combination of modeling and experimental data. Experimental and computational users are encouraged to attend. For hands-on work, participants should be comfortable using a Linux command line environment and should bring their own laptop. Participants are encouraged to bring their research problems for diagnostics.

9:00 – 3:00 CNM Short Course C: Building 212, Room A157 and Building 212, D-Wing Microscopy Labs
Transmission Electron Microscopy (TEM) for Materials Science
Instructors: Yuzi Liu and Jianguo "JG" Wen (CNM)

This course targets the researcher with an entry to medium level knowledge of transmission electron microscopy (TEM). (S)TEM characterization and Aberration-corrected S/TEM for advanced energy material techniques will be introduced along with real examples. A demo of these techniques will follow the presentation.

APS Satellite Workshops

8:00 – 4:30 APS Satellite Training Course: Building 401, Room A5000

SAXS Software Software Packages Irena and Nika (Day 1)

Instructor: Jan Ilavsky (Argonne National Laboratory)

Successful small-angle x-ray scattering (SAXS, SANS) experiment requires appropriate data reduction and analysis tools. Igor Pro based packages Nika (for SAXS data reduction) and Irena (for SAS = SAXS/SANS/USAXS/USANS data analysis) were developed during the last 15 years at the APS. They are already being used widely for material science SAS at the APS and at other facilities worldwide. These tools are commonly included in syllabus of "Beyond Rg Materials" - SAXS short course organized semi-annually by APS SAXS SIG. However, the main audience of this SAXS short course is new SAXS users, starting with their own SAXS program and therefore it focuses more heavily on experiments, theory etc. The time devoted in this course for software is insufficient for experienced experimenters interested in complex software applications.

Therefore, the APS SAXS Special Interest Group (SIG) is organizing this specialized, hands-on, course specifically on the SAS software Nika and Irena. The course will be taught by the software author, Jan Ilavsky, APS staff member. In order to provide high educational value, the number of participants will be limited to 20. Participants are expected to have a high level of SAS experience and bring their own computers (Windows or OSX). In addition, they are encouraged to bring their own SAS experimental results.

Daily Schedule

8:00 Welcome coffee and continental breakfast

8:30 Course begins

~10:30 Break

12:00 Lunch (1 hour on own)

~2:30 Break

4:30 Adjourn

Working Agenda: Thursday, May 9

1. Installation of both packages/verification of functionality
2. Nika data reduction:
    a. Orientation in the program
    b. Calibration/geometry
    c. Mask design
    d. Data processing, sector and circular data reduction
    e. GI geometry, line profile, profile around ellipse…
    f. Programing for Nika (look up functions)
3. Irena data analysis:
    a. Orientation in the program

8:15 – 4:00 APS Satellite Training Course: Building 401, Room A1100

XANES and High-energy Resolution Fluorescence Detection (HERFD) XANES

Instructor: Matt Newville (GSECARS) and Josh Kas (University of Washington)

This training course will provide a description of measurement methods for high-resolution XANES and on data processing and analysis methods of XANES and resonant inelastic scattering. The course includes a mixture of practical training of analysis methods with talks on applications and advanced methods.

Daily Schedule

8:15 Welcome coffee and continental breakfast

9:00 Course begins

~10:30 Break

12:00 Lunch (1 hour on own)

~2:30 Break

4:00 Adjourn

Morning Session: Empirical Analysis for XANES + Methods
(Matthew Newville, University of Chicago)

1. Introduction, Data Processing, Over-absorption corrections.
2. Principal Component Analysis
3. Linear combination fitting
4. Multivariate / dimensionality reduction with LASSO-based supervised learning.
5. Fitting Pre-edge peaks

Afternoon Session: Theoretical Simulations of XANES + Methods
(Josh Kas, University of Washington)

Friday, May 10

APS Satellite Workshops

8:00 – 4:30 APS Satellite Training Course: Building 401, Room A5000
SAXS Software Software Packages Irena and Nika (Day 2)
Instructor: Jan Ilavsky (Argonne National Laboratory)

Daily Schedule

8:00 Welcome coffee and continental breakfast

8:30 Course begins

~10:30 Break

12:00 Lunch (1 hour on own)

~2:30 Break

4:30 Adjourn

Working Agenda: Friday, May 10

3. Irena data analysis, continued:

    b. Import of data

    c. Data plotting

    d. Data manipulation

    e. Unified fit, advanced analysis

    f. Size distribution

    g. Modeling tools

    h. Scattering contrast calculator

    i. Analytical tools

    k. SA Diffraction tool

    l. Reflectivity tool

    m. other tools…until end of the day.

8:15 – 5:30 APS Satellite Training Course: Building 401, Room A1100

X-ray Absorption Spectroscopy Simulations using FDMNES

Organizers: Yves Joly (Institut Néel, CNRS, Grenoble, France) and Chengjun Sun (ANL)

8:15 Welcome coffee and continental breakfast

9:00 Lecture on X-ray Matter Interaction

9:45 Break

10:00 Application for XANES, X-ray Raman and Resonant Diffraction

11:00 Break

11:15 Presentation of the FDMNES Software

11:30 Practical – XANES

12:30 Lunch (on own)

2:00 Practical – Dichroism, Resonant Diffraction, Surface Resonant Diffraction, X-ray Raman

3:30 Break

3:45 Practical on Examples Proposed by the Participants

5:30 Adjourn

Participants must bring a laptop. A package including the software (Windows, Mac or Linux), documentation and set of examples will be provided. Software to plot spectra (Origin, Kaleidagraph, etc.) is required.

GENERAL SESSION ABSTRACTS

APS PLENARY

X-ray Thermal Diffuse Scattering: History, Advances, and Opportunities

Tai C. Chiang
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801

I will tell a story about my group's research program on utilizing thermal diffuse scattering (TDS) to investigate phonon properties of crystals. Right around the time the Advanced Photon Source opened its door to users, we were trying to perform surface diffraction with a transmission geometry, hoping to develop an efficient method for determining the atomic structure of reconstructed surfaces. Instead, we found beautiful TDS patterns from the bulk, which overwhelmed the surface signals. TDS arises from scattering by lattice vibrations (phonons). Debye realized in 1913 that lattice vibrations reduce the diffraction peak intensities (by the Debye Waller factor) and the lost intensities are dispersed into a diffuse but feature-rich TDS background. A number of pioneers in x-ray diffraction recognized that TDS could be useful for phonon studies, but early experiments based on x-ray tubes were inefficient and impractical. With the advent of neutron scatting in the 1950s, the x-ray TDS method was largely abandoned and forgotten. At APS, high-quality 2D TDS patterns over a wide range of momentum transfer could be acquired in seconds, but it took us quite a while to develop the mathematical tools needed to extract useful information from the data. I will show some examples to illustrate the technical progress and the utility of TDS for studies of phonons, soft modes, and phase transitions in various materials including tiny samples, which are difficult for neutron scattering. I will comment on what we are working on now, including time-resolved studies following pulsed excitations.

I wish to thank the people who made APS a reality and my group members, colleagues, the UNICAT team (with members from the University of Illinois, Oak Ridge, NIST, Allied Signal, and UOP), and APS staff who participated in and/or helped with this research.

APS PLENARY

X-ray Imaging and Spectroscopy of the Brain

Yulia Pushkar
Department of Physics, Purdue University, West Lafayette, IN 47906

The increasing prevalence of neurodegenerative diseases such as Alzheimer's (AD) and Parkinson's (PD) diseases is a major public health as well as economic concern in the USA and other developed countries. Currently, no treatment is available to slow the progression of these diseases and the aging population, which is disproportionately affected by these diseases, place an increasing strain on the economy. Recent research implicates trace elements (such as Mn, Fe, Cu and Zn) neurotoxicity in the etiologies of Alzheimer's (AD) and Parkinson's (PD) diseases but the molecular mechanisms are mostly unknown. The number of experimental techniques that can measure metal distribution and speciation in the brain is limited.

I will present x-ray fluorescence imaging, a method for quantitative analysis of elemental distribution in the brain; and x-ray diffraction imaging, which is sensitive to structural features in key elements of a healthy brain, such as myelin and neurofilaments—as well as pathological aggregates—such as plaques, Lewy bodies, and neurofiblillary tangles. Using XRF we studied Mn distribution in rat model of occupational Mn exposure [1–4]. We found that globus pallidus and substantia nigra compacta are areas in the brain that accumulate most Mn. Imaging the Mn distribution in dopaminergic neurons of exposed rats we determined that intracellular Mn range between 40–200 micromolar; concentrations as low as 100 micromolar have been observed to cause cell death. This is a first potentially direct link between Mn exposure and Parkinson's disease.

Via XRF analysis of healthy rodent brains have discovered localized Cu-rich aggregates in astrocytes of the subventricular zone with Cu concentrations in the hundreds of millimolar [5–7]. Based on a [S]/[Cu] ratio and x-ray absorption spectroscopy, metallothionein was proposed as a binding protein. An analysis of metallothionein(1,2) knockout mice by XRF shown decrease in number of Cu containing aggregates but these were not eliminated indicating alternative pathways for aggregates formation.

[1] Sullivan, B.; Robison, G.; Kay, M.; and Pushkar, Y. (2016). "Mn exposure does not affect neurogenesis," **152**(2): 257–261.

[2] Robison, G.; Sullivan, B.; Cannon, J.R.; and Pushkar, Y. (2015). "Identification of dopaminergic neurons of the substantia nigra pars compacta as a target of manganese accumulation," *Metallomics* **7**(5): 748–755.

[3] Robison, G.; Zakharova, T.; Fu, S.; Jiang, W.D.; Fulper, R.; Barrea, R.; Zheng, W.; and Pushkar, Y. (2013). "X-ray fluorescence imaging of the hippocampal formation after manganese exposure," *Metallomics* **5**(11): 1554–1565.

[4] Robison, G.; Zakharova, T.; Fu, S.; Jiang, W.; Fulper, R.; Barrea, R.; Marcus, M.A.; Zheng, W.; and Pushkar, Y. (2012). "X-ray Fluorescence Imaging: A New Tool for Studying Manganese Neurotoxicity," *PLoS One* **7**(11).

[5] Sullivan, B.; Robison, G.; Pushkar, Y.; Young, J.K.; and Manaye, K.F. (2017)."Copper accumulation in rodent brain astrocytes: A species difference," **39**: 6–13.

[6] Sullivan, B.; Robison, G.; Osborn, J.; Kay, M.; Thompson, P.; Davis, K.; Zakharova, T.; Antipova, O.; and Pushkar, Y. (2017). "On the nature of the Cu-rich aggregates in brain astrocytes," **11**: 231–239.

[7] Pushkar, Y.; Robison, G.; Sullivan, B.; Fu, S.X.; Kohne, M.; Jiang, W.; Rohr, S.; Lai, B.; Marcus, M.A.; Zakharova, T.; and Zheng, W. (2013). "Aging results in copper accumulations in glial fibrillary acidic protein-positive cells in the subventricular zone," *Aging Cell* **12**(5): 823–32.

APS PLENARY

On the Use of Automatic Differentiation for Phase Retrieval

Saugat Kandel[1], S. Maddali[2], Ming Du[3], Marc Allain[4], Stephan O. Hruszkewycz[2], Chris Jacobsen[5,6,7], and Youssef Nashed[8]

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The recent rapid development in coherent diffraction imaging (CDI) methods has enabled nanometer-resolution imaging in a variety of experimental modalities. Image reconstruction with such CDI methods involves solving the phase retrieval problem, where we attempt to reconstruct an object from only the amplitude of its Fourier transform. This can be framed as a nonlinear optimization problem which we can solve using a gradient-based minimization method. Typically, such approaches use closed-form gradient expressions. For complex imaging schemes, deriving this gradient can be difficult and laborious. This restricts our ability to rapidly prototype experimental and algorithmic frameworks.

In this work, we use the *reverse-mode automatic differentiation* method to implement a generic gradient-based phase retrieval framework. With this approach, we only need to specify the physics-based forward propagation model for a specific CDI experiment; the gradients are exactly calculated automatically through a sequential application of the chain rule in a *reverse pass* through the forward model. Our gradient calculation approach is versatile and can be straightforwardly implemented through various deep learning software libraries (TensorFlow, Pytorch, Autograd, etc.), allowing for its use within state-of-the-art accelerated gradient descent algorithms. We demonstrate the generic nature of this phase retrieval method through numerical experiments in the transmission (far-field and near-field), Bragg, and tomographic CDI geometries.

APS PLENARY

Simulating Meteor Impacts in the Diamond Anvil Cell

Melissa Sims[1], Melinda Rucks[1], Sergey Lobanov[1], Jordan Young[1], Kip Daly[1], Anna Pahmakova[2], Zuzana Konopkova[3], Hanns-Peter Liermann[2], Ross Hrubiak[4], Yue Meng[4], Matthew L. Whitaker[1,5], Timothy D. Glotch[1], and Lars Ehm[1,5]

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Impact cratering is important in planetary body formation and evolution [1,3]. The pressure and temperature conditions reached during impacts are classified using systems [4–6] that stem from 1) petrographic deformation features observed in the impactite and 2) the presence of high pressure mineral phases. However, the effects of kinetics and strain-rate on deformation features and high-pressure phases are relatively unconstrained [7]. We completed room temperature, 300°C, and laser-heated rapid compression and decompression membrane and dynamic diamond anvil cell (mDAC and dDAC) experiments with *in situ* x-ray diffraction [2]. We studied olivine ($(Mg, Fe)_2 SiO_4$) and plagioclase ($NaAlSi_3O_8$-$CaAl_2Si_2O_8$). The compression and decompression rates were between 0.04–81.0 GPa/s up to pressures around 50 GPa. The compression rates allow us to observe deformation and transformation mechanisms as well as thermodynamic effects in detail. In plagioclase, we identify a specific mechanism for amorphization and define decompression effects on nucleation. In olivine, we suggest what mechanisms lead to the deformation features observed in shocked samples. These experiments have allowed us to identify some of the complex interactions that likely play a role in natural events and are previously unexplored.

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APS PLENARY

Peeking into Excited State Trajectories with Pulsed X-rays: A Journey of Two Decades

Lin X. Chen

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I will give a very brief reflection of 20 years in taking snapshots of photoexcited molecular species in solar energy conversion processes at the APS and beyond. Then I will use two recent examples to demonstrate how x-ray spectroscopies from the APS can decipher both electronic and nuclear geometry in the ground and excited state molecular species.

Electronic Structures of Metal Centers in an OER Catalyst Model. One of the challenges in solar fuels generation is generating multiple redox equivalents for the oxygen evolution reaction (OER) (i.e., $2H_2O \rightarrow O_2+4H^++4e^-$) that is a four-electron, four-proton coupled process. In collaboration with Nocera Group, we used a combination of *in situ* and *ex situ* x-ray absorption and emission spectroscopies as well as quantum mechanical calculations on OER thin films and their molecular and heterogeneous inorganic analogs. These studies provided insights into the electronic structures of the high-valent states involved in the mechanisms of O-O bond formation and for the high-valent states to drive the bond-forming and bond-breaking steps of OER reactions. We employed complementary x-ray spectroscopies, x-ray absorption (XAS) and 1s3p resonant inelastic x-ray scattering (K_β RIXS), to effectively extract Co(IV) contributions within a spectroscopically active background. Co K- and L-edge x-ray absorption directly probe the 3d-manifold of effectively localized Co(IV), providing a handle on the covalency of the dπ-based redox active molecular orbital (MO) of Co_4O_4. We also probed the doubly oxidized $Co(III)_2(IV)_2$ state of the Co_4O_4 cluster, which features a cofacial $Co(IV)_2$ site and is thus a molecular model of the active site in Co-OEC.

Electron and Energy Relays in the Excited State Supramolecular Dinuclear Transition Metal Complexes. The rational design of multinuclear transition metal complexes (TMCs) for photochemical catalysis of homogeneous and/or heterogeneous multi-electron reactions (e.g., for producing solar fuels) requires a detailed understanding of the often unique and convoluted excited state charge and energy transfer dynamics in this class of compounds. Using combined optical and x-ray transient spectroscopic measurements, excited state electron electron relays in tetrapyridophenazine-bridged heteroleptic dinuclear Cu(I) bis(phenanthroline) complexes have been investigated as an exemplary system.

CNM PLENARY

Visualizing Novel Quantum States of Matter

Ali Yazdani

Class of 1909 Professor of Physics and Director, Princeton Center for Complex Materials, Princeton University, Princeton, NJ 08544

Spectroscopic mapping with the scanning tunneling microscope (STM) at low temperatures allows us to explore quantum materials in an unprecedented fashion. In this talk, I will describe a few studies at the forefront of research in quantum condensed matter physics. One area of research is related to topological quantum computing in which we have used the STM to visualize an exotic quasi-particle called a Majorana zero mode. I will also describe STM studies in very high magnetic field in which we provide direct visualization of quantized electrons' Landau orbits, which that underlie the formation topological quantum Hall state. I will close with an outlook of some of the exciting problems in the condensed matter physics, which can be addressed using STM spectroscopic mapping techniques.

CNM PLENARY

Expanding the Scope of Nanobeam Diffraction: Dynamical Diffraction in Epitaxial Electronic Materials

Paul G. Evans

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Epitaxial electronic materials include a thin film or nanostructure that shares key aspects of its crystallographic structure with a thick underlying substrate. In key applications of these epitaxial materials in the development of semiconductor quantum computing, the control of this structure at the scale of tens to hundreds of nanometers has been an important challenge. Semiconductor quantum computing devices based on heterostructures formed in the AlGaAs/GaAs system involve thin epitaxial layers with tiny lattice mismatches

on the order of 10^{-4} or smaller and rely on the formation of qubits defined at the lateral scale of tens of nanometers. The further mechanical distortion of these layers during the formation of devices causes significant electronic perturbations due to the piezoelectric and deformation potential effects. Ultimately, the mechanical distortion and the accompanying electronic perturbation affects the operation of devices. It has been challenging, however, to characterize the mechanical distortion of these epitaxial layers, in part because the close lattice match between the substrate and the thin film has posed a difficult problem for x-ray nanobeam diffraction techniques. We have found that this problem can be addressed through the development of new nanobeam diffraction methods in which dynamical diffraction simulations are employed to interpret the complex diffraction patterns arising from latticed-matched heterostructures [1].

Nanobeam diffraction studies of lattice-matched GaAs/AlGaAs quantum computing devices reveal mechanical distortions due to device fabrication, including from the residual stress and thermal expansion coefficient mismatch associated with metallic electrodes [2,3]. This new understanding the magnitude and role of these effects has the potential to allow the design of improved device geometries and potentially to lead to devices in which strain, in addition to electrostatic effects, is used to define quantum devices.

Beyond quantum computing structures, similar dynamical diffraction effects appear in problems associated with ferroelectric domains and domain boundaries in epitaxial $BaTiO_3$ thin films and in strain sharing effects in nanoscale complex oxides [4].

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CNM PLENARY

Development and Understanding of the Origin of Irreversibility in Layered Transition-metal Oxide Cathode Material for Sodium Ion Batteries

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Sodium ion batteries are attractive alternative energy storage technology to lithium-ion batteries due to its low-cost. There has been growing attention in developing new cathode materials for sodium ion batteries. The Iron-based layered oxide cathode is of significant interest due to the low-cost, abundant, environmentally-friendly material selection. The O3-type layered $Na(Ni_xFe_yMn_z)O_2$ ($0 < x, y, z < 1$) (NFM) cathode materials have attracted great interest in sodium-ion batteries due to the abundance and cost of raw materials and their high specific capacities. However, the cycling stability and rate capability at high voltages (> 4.0V) of these materials remains an issue. In this work, we investigated the effect of Li substitution in NFM cathode and successfully synthesized a Li-substituted layered-tunneled (O3-spinel) intergrowth cathode (LS-NFM) to address these issues.

The remarkable structural compatibility and connectivity of the two phases were confirmed by x-ray diffraction (XRD), selected area electron diffraction (SAED) and high resolution transmission electron microscopy (HRTEM). The LS-NFM cathode exhibits enhanced cycling stability as well as rate capability compared to the un-doped NFM cathode. The enhanced rate capability of LS-NFM can be explained by the significantly increased effective Na^+ diffusivity measured by galvanostatic intermittent titration technique (GITT) compared to the un-doped control NFM cathode, which can be ascribed to the improved charge transport kinetics through shortened diffusion path by direct connection between the 3D channels in the spinel phase and 2D channels in the layered phase. The results from *ex situ* hard/soft x-ray adsorption spectroscopy (XAS) suggest that the capacity of LS-NFM cathode is mainly associated with the Ni^{2+}/Ni^{4+} redox couple, and slightly from the Fe^{3+}/Fe^{4+} redox couple. We also investigated the

origin of irreversibility of un-doped NFM cathode materials. It was found that the irreversibility became pronounced and the electrochemical performance became limited with the increase of either Fe composition or the upper cutoff potential in these materials.

CNM PLENARY

Hybrid Organic-inorganic Perovskites: From Anisotropic Excitons to Soft Crystal Lattice

Peijun Guo[1], Constantinos C. Stoumpos[2], Jue Gong[3], Arun Mannodi-Kanakkithodi[1], Yi Xia[1], Lingling Mao[2], Duyen H. Cao[4], Sridhar Sadasivam[1], John B. Ketterson[5], Pierre Darancet[1], Maria K.Y. Chan[1], Tao Xu[3], Mercouri G. Kanatzidis[2], and Richard D. Schaller[1]

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Hybrid organic-inorganic perovskites are solution-processed, scalable materials exhibiting remarkable optoelectronic properties such as strong light absorption, defect tolerance, and long carrier lifetimes. I will describe how electronic excitations in these materials are coupled to and influenced by the vibrational degrees of freedom of the organic and inorganic sublattices, investigated using an array of optical spectroscopic techniques. The unique soft nature of the lead-halide octahedral framework gives rise to dynamic fluctuations in the electronic bandgap, which distinguishes hybrid perovskites from traditional inorganic semiconductors. Furthermore, strong quantum confinement can be easily imparted to hybrid perovskites with the use of organic spacer-molecules, leading to exotic dispersion relation and enhanced light-emitting properties. Our results demonstrate that hybrid materials consisting of distinct sub-lattices can allow for dramatically enhanced light absorption, emission and charge carrier collection at various time- and length-scales.

CNM PLENARY

Fabrication, *in situ* Biasing, Electron Holography and Elemental Analysis of Patterned and Unpatterned TiO_2 Thin Films

Frank Barrows[1,2], Yuzi Liu[3], Charudatta Phatak[1], Saidur Bakaul[1], and Amanda Petford-Long[1,4]

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TiO_2 is a metal oxide that can undergo resistive switching, a reversible change between high and low resistance states by application of a voltage bias. This behavior has promising applications in neuromorphic computing and nonvolatile memory. In order to gain a deeper understanding of the mechanism behind reversible switching and electric breakdown in TiO_2 we have fabricated samples for *in situ* biasing and Transmission Electron Microscopy, (TEM). Additionally, we have patterned thin films of TiO_2 on the nanoscale as a means to gain additional insights into the reversible breakdown through *in situ* biasing.

I will present details of the fabrication process we developed at the Center for Nanoscale Materials, (CNM). This includes both the process to pattern TiO_2 thin films and the preparation of thin films for *in situ* biasing in TEM. In order to pattern TiO_2 , we perform sequential infiltration synthesis of Al_2O_3 into block copolymers to make a patterned film of Al_2O_3 on top of thin films of TiO_2. Using reactive ion etching we transfer the Al_2O_3 pattern into the TiO_2 thin film. To prepare these patterned and unpatterned samples for *in situ* biasing we use electron beam lithography to write electrodes on top of the TiO_2 thin films. Finally, we use wet etching to back etch SiN windows into our substrate. Additionally, I will present results from *in situ* biasing experiments. Using electron holography and electron energy loss spectroscopy (EELS) in the CNM, we have observed irreversible changes in our thin films during our biasing experiments. I will compare these results in the patterned and unpatterned TiO_2 films.

This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Science, Materials Sciences and Engineering Division. Use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

WORKSHOP AGENDAS AND ABSTRACTS

Tuesday, May 7

WK1 Joint APS/CNM: Driving Scientific Discovery with Artificial Intelligence, Advanced Data Analysis, and Data Management in the APS-U Era

Location: Building 402, Room E1100/1200

Time: 8:45 – 5:00

Organizers: Nicholas Schwarz (APS/ANL), Chengjun Sun (APS/ANL), and Mathew Cherukara (CNM/ANL)

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

These advances are expected to drastically increase the amount and complexity of data generated by instruments at the APS, especially in the areas of coherence driven, imaging, high-energy scattering, advanced x-ray spectroscopy, and multi-modal techniques enabled by APS-U era facilities. However, methods for understanding data have not always kept pace. Manual analysis and management of data is too time consuming and cumbersome for large, complex datasets. State-of-the-art mathematics and computer science tools will help automate the understanding process. The scientific mission of the APS-U era facility will only be achieved by coupling the capabilities of the facility with advanced data analysis and data management resources.

For example, machine learning methods including deep learning methods, have been employed to accelerate data analysis for advanced x-ray spectroscopy and time-resolved x-ray and electron imaging, to design new molecular structures, to automate manufacturing and to accelerate the materials design loop. This workshop is organized to discuss the state-of-the art and potential of artificial intelligence, and data analysis and management for the APS and CNM. It is expected to provide an opportunity for academics, R&D scientists in industry, and students to exchange ideas and think creatively about new avenues for collaborations.

Topics include, but are not limited to:

- Data analysis and machine learning algorithms and software
- Experiment design and real-time experiment steering
- Deep learning approaches for inverse imaging problems, and feature detection and labeling
- Machine learning to accelerate high-throughput computational x-ray absorption spectroscopy
- Data driven material selection and synthesis, property prediction and inverse design of materials
- On-demand utilization of high-performance computing resources
- Data management and data collaboration workflow tools
- Deep learning at scale
- Introduction to machine learning for x-ray diffraction, spectroscopy, and imaging

The goal is to elaborate on how users can benefit from advanced data analysis and management techniques, and to identify needs to enable new scientific discovery in the APS-U era.

8:45 – 9:00	Opening Remarks
9:00 – 9:30	TBD *coming soon*
9:30 – 10:00	Elise Jennings (Argonne National Laboratory) *Scientific Machine Learning at Argonne Leadership Computing Facility*
10:00 – 10:30	Break
10:30 – 11:00	Shuai Liu (University of California-Berkeley, Lawrence Berkeley National Laboratory) *Driving Scientific Discovery with Artificial Intelligence, Advanced Data Analysis and Data Management in the APS-U Era*
11:00 – 11:30	TBD *coming soon*
11:30 – 12:00	Nouamane Laanait (Oak Ridge National Laboratory) *Decoding Inverse Imaging Problems in Materials with Deep Learning and Supercomputing*
12:00 – 1:00	Lunch
1:30 – 2:00	Shyam Dwaraknath (Lawrence Berkeley National Laboratory) *The Materials Project: Conception to Confirmation in a Virtual Lab*
2:00 – 2:30	John Rehr (University of Washington) *High-throughput Computational X-ray Absorption Spectroscopy*
2:30 – 3:00	Maria Chan (Argonne National Laboratory) *Combining Characterization and Modeling Data for the Determination of Nanoscale Structures*
3:00 – 3:30	Break
3:30 – 4:00	Saugat Kandel (Northwestern University and Argonne National Laboratory) *Learning Phase Retrieval with Backpropagation*
4:00 – 4:30	Daniela Ushizima (Lawrence Berkeley National Laboratory) *Thin Film Structure Identification through Convolutional Neural Networks Applied to Scattering Patterns*
4:30	Discussion and Close Out

WK1

Scientific Machine Learning at Argonne Leadership Computing Facility

Elise Jennings
Argonne National Laboratory, Lemont, IL 60439

Scientific machine learning has the potential to transform science and energy research and has found a broad use across DOE user facilities. Scientific progress and discovery is being driven by massive data together with optimized software for predictive models and algorithms running on heterogeneous high-performance computing platforms. The ALCF data science program (ADSP) supports projects which push the state-of-the-art in data-centric and data-intensive computing; as well as in machine learning, deep learning, and other AI methods at scale. I will discuss the data science research at ALCF and give an overview of current ADSP projects relevant to the APS.

WK1

Driving Scientific Discovery with Artificial Intelligence, Advanced Data Analysis and Data Management in the APS-U Era

Shuai Liu
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Lawrence Berkeley National Laboratory, Berkeley, CA 94720

X-ray scattering has a variety of applications in science to investigate the structure of different materials systems. However, it remains challenging to analyze large-scale x-ray scattering data in a high-throughput and effective fashion. We propose to approach this problem using machine learning to categorize the data and to determine the underlying structure of the materials. Here we propose a hierarchical categorization method to cluster the features in the x-ray scattering data and to manage large-scale experimental data. Moreover, this method is applied to several *in situ* experimental systems in order to detect the structure transitions automatically. Second, we illustrate a machine learning methodology to classify the underlying materials structure from x-ray scattering data. The machine learning model is trained using data generated from the high performance GISAXS (HipGISAXS) simulation package. This methodology is applied to binary superlattices in thin films to characterize the crystal structure. Finally, we introduce a new neural network architecture, which proved to be more effective than conventional convolutional neural networks looking at x-ray scattering and XRD datasets.

WK1

Decoding Inverse Imaging Problems in Materials with Deep Learning and Supercomputing

Nouamane Laanait
Computational Sciences and Engineering Division,
Oak Ridge National Laboratory, Oak Ridge, TN 37830

Modern Scanning Transmission Electron Microscopes (STEM) provide sub-Angstrom beam sizes, high spatial coherence and fast frame rates. In principle, STEM imaging could enable characterization of local materials properties at unit-cell spatial resolutions. The fundamental challenge to a quantitative analysis of scattering data in the STEM, however, has remained the same for 80 years, namely an intractable inverse problem where dynamical scattering is prevalent. In this talk, we present a few examples where a deep learning approach to this inverse problem in the STEM was successfully applied and discuss its advantages and current limitations. First, we show that deep convolutional neural networks (DCNN), trained on multislice simulations, learn to accurately predict the 3-D oxygen octahedral rotations in complex oxides from annular bright-field (ABF) images, with sub-degree accuracy and unit-cell spatial resolutions. Second, we show that distributed deep learning, implemented on Oak Ridge National Lab's Summit supercomputer (and scaled to 10,000 GPUs) can successfully "invert" coherent convergent-beam electron diffraction (CBED) data to uncover the projected atomic potential for a limited set of material classes, with sub-Angstrom spatial resolutions.

WK1

The Materials Project: Conception to Confirmation in a Virtual Lab

Shyam Dwaraknath
Lawrence Berkeley National Laboratory, Berkeley, CA 94720

The materials project (MP) is an open searchable database of computed materials properties to enable a transition to materials by design. MP currently documents over 133,000 materials and a range of associated properties from the electronic structure, elastic tensor, dielectric tensors, piezoelectric tensors, phonons, substrates recommendations, and more. This rich data set enables scientists to search for materials with appropriate functionality and identify those that are the most likely to be thermodynamically stable both chemically and dynamically. Building on this, the local spectroscopy data initiative (LSDI) is an effort in MP to build a database of computed x-ray absorption spectroscopy (XAS) spectra and tools to enable researchers to investigate the characterizability of a material. Only a small percentage of the materials community can take full advantage of emergent capabilities at light sources.

Enabling broad access to simulated data for materials discovery will greatly increase the user-base at APS by allowing researchers to "experiment" *in silico*; greatly reducing the necessary expertise and resource risks. While this data-set provides a powerful first step in democratizing XAS, it also creates new challenges. For instance, the over 600,000 site-specific XAS spectra at LSDI makes spectral matching in a traditional human-in-the-loop fashion rather difficult. To solve these big-data challenges, the LSDI is also developing tools to enable integration into materials discovery pipelines and eventually enable automatic online identification of local environments.

WK1

High-throughput Computational X-ray Absorption Spectroscopy

John J. Rehr[1,2], Joshua J. Kas[1], Fernando D. Vila[1], Kiran Mathew[3], Chen Zheng[4], Donald Winston[5], Chi Chen[4], Yiming Chen[4], Alan Dozier[6], Shyam Dwaraknath[3], Shyue Ping Ong[4], and Kristin A. Persson[3]

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Modern electronic structure theory and computational methods now permit efficient calculations of many ground state materials properties, as exemplified by results from the Materials Project [1]. Complementary advances in the theory of excited states have led to efficient methods for calculations of x-ray and electron spectroscopies (e.g., the real-space Green's multiple scattering theory in the FEFF9 code [2]). Here we discuss these developments and their application to high throughput calculations of x-ray absorption spectra [3]. In particular, a database of computed spectra has been developed which currently contains over 800,000 K-edge spectra for over 40,000 materials, which has also been used in ensemble-learned matching of near edge spectra [4]. The database is freely available from the Materials Project [1], and extensions to other spectra are in progress.

This work was a product of the Data Infrastructure Building Blocks (DIBBS) Local Spectroscopy Data Infrastructure project funded by NSF under Award 1640899. The FEFF code development is supported primarily by the DOE Office of Science, BES Grant DE-FG02-45623 (JJR,JJK,FDV). Computational resources were provided by the NSF DIBB funding and the Triton Shared Computing Cluster (TSCC) at the University of California, San Diego. The online data and search capabilities were funded by the DOE Office of Science, BES, MSE Division under Contract No. DE-AC02-05-CH11231: Materials Project program KC23MP.

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WK1

Combining Characterization and Modeling Data for the Determination of Nanoscale Structures

Maria Chan

Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439

Determining the atomistic structures in the nanoscale is a challenging problem. Although there are both experimental and computational methods to determine these nanoscale structures, they both possess limitations. We developed the fully automated nanoscale to atomistic structure from theory and eXperiment (FANTASTX) code to overcome the limitations of either by combining both experimental and computational data, with the help of machine learning. The approach will be illustrated using x-ray and electron-microscopy data, combined with first principles density functional theory (DFT), or empirical force field (FF) guidance, and machine learning tools.

WK1

Learning Phase Retrieval with Backpropagation

Youssef S.G. Nashed[1], Saugat Kandel[2], Ming Du[3], and Chris Jacobsen[4,5]

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Synchrotron radiation light source facilities are leading the way to ultrahigh resolution x-ray imaging. High resolution imaging is essential to understanding the fundamental structure and interaction of materials at the smallest length scale possible. Coherent diffraction imaging (CDI) achieves nanoscale imaging by replacing traditional objective lenses by pixelated area detectors and computational image reconstruction. We present our work for solving CDI reconstruction problems through fitting a physics based model to measured data. The model parameters are learned in a similar manner to deep neural networks, utilizing the backpropagation method as implemented in Google TensorFlow package. This approach has advantages in terms of speed and accuracy compared to current state of the art algorithms, and demonstrates re-purposing the deep learning backpropagation algorithm to solve general phase retrieval problems that are prevalent in lensless microscopy research.

WK1

Thin Film Structure Identification through Convolutional Neural Networks Applied to Scattering Patterns

Shuai Liu[1,2], Charles N. Melton[1], Singanallur Venkatakrishnam[3], Ronald J. Pandolfi[1], Guillaume Freychet[1], Dinesh Kumar[1], Haoran Tang[2], Alexander Hexemer[1], and Daniela M. Ushizima[1,2]

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Nano-structured thin films have a variety of applications from waveguides, gaseous sensors to piezoelectric devices. Among the methods to investigate such materials, grazing incidence small angle x-ray scattering (GISAXS) consists of a surface-sensitive technique that enables probing complex morphologies ranging from the fields of polymer and soft matter science, to hard-condensed matter. One challenge is to determine structure information from these scattering patterns alone. Our recent work showcase how GISAXS images work as signatures, which depend on the size, shape and arrangement of nanostructured components, ultimately enabling the classification of thin films.

The CNN-based classification scheme categorizes seven combinations of 3D nanoparticle lattice orientations from simulated x-ray scattering data based on observable features in scattering patterns. Training data are obtained using HipGISAXS [1] scattering simulator. Several million scattering patterns were generated for seven different nanoparticle crystal lattices at various orientations. We verify the robustness of the CNN by subjecting the training data to various noise sources that simulate typical data artifacts. This talk presents details about work published at the Materials Research Society Communications, Cambridge Press [2]. It describes the design of multiple Convolutional Neural Networks to classify nanoparticle orientation in a thin film by learning scattering patterns. The network was trained on several thin films with a success rate of 94%. We demonstrate CNN robustness under different artifacts as well as show the potential of our proposed approach as a strategy to decrease scattering pattern analysis time.

This work was supported by the Center of Advanced Mathematics for Energy Research Applications (CAMERA) through the Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and the Early Career Program. This research is funded in part by the Gordon and Betty Moore Foundation through Grant GBMF3834 and by the Alfred P. Sloan Foundation through Grant 2013-10-27 to the University of California, Berkeley.

[1] S.T. Chourou, A. Sarje, X.S. Li, E.R.Chan, and A. Hexemer (2013). "HipGISAXS: a high performance computing code for simulating grazing-incidence x-ray scattering data," *J. Appl. Crystallogr.* **46**: 1781–1795. https://hipgisaxs.github.io/.

[2] S. Liu, C. Melton, S. Venkatakrishnam, R. Pandolfi, G. Freychet, D. Kumar, H. Tang, A. Hexemer, and D. Ushizima (2019). "Convolutional Neural Networks for Grazing Incidence X-ray Scattering Patterns: Thin Film Structure Identification," Special Issue on Artificial Intelligence, Materials Research Society, Cambridge Press (accepted).

Wednesday, May 8

WK2 Joint APS/CNM: Topological Quantum Information Science

Location: Building 401, Room A1100

Time: 9:00 – 5:30

Organizers: Yue Cao (MSD), Pierre Darancet (CNM), Nathan Guisinger (CNM), Jessica McChesney (APS), Subramanian Sankaranarayanan (CNM), Hua Zhou (APS)

The conceptual design and experimental observation of topological phases of matter have opened up new avenues for Quantum Information Science. In particular, topologically protected states can feature longer electron coherence time, and offer control over dissipation channels via the time and space group symmetry of materials.

Despite the tremendous success of the past decade in predicting, synthesizing, and characterizing topological materials, many topological phases of matter central to quantum information science, such as Majorana fermions and topological bosons have yet to be observed. Moreover, realistic application of topological materials will require protocols that precisely control the material properties responsible for the propagation of information (e.g., the flow of spin current, or the braiding of Majorana fermions). This workshop will address the main progress and challenges in the research of topological materials, and cover the entire life cycle of these studies, from computational design, experimental realization, to control methods and device schemes towards topological devices. Speakers will feature major players in all the aforementioned sub-areas of research.

9:00 – 9:15 Yue Cao (Argonne National Laboratory)
Opening Remarks

9:15 – 9:30 John Mitchell (Argonne National Laboratory)
Welcome

Session 1: Topological Materials: Where Do We Find Them? (Pierre Darancet)

9:30 – 10:05 Ivar Martin (Argonne National Laboratory)
Hamiltonian Engineering with Majorana Modes

10:05 – 10:40 Aash Clerk (University of Chicago)
Photonic and Bosonic Analogues of Topological Superconductors

10:40 – 11:00 Break

Session 2: Topological States in the Bulk (Nathan Guisinger)

11:00 – 11:35 John Mitchell (Argonne National Laboratory)
Putative Topological Features in $Co_{1/3}NbS_2$ and Pd_3Pb

11:35 – 12:10 Ni Ni (University of California, Los Angeles)
Experimental of Topological Materials

12:10 – 1:30 Lunch

Session 3: Artificial Topological States on the Surface and Interface (Hua Zhou)

1:30 – 2:05 Seongshik Oh (Rutgers, the State University of New Jersey)
Tunable Proximity-coupled Topological Superconductor Heterostructures for Quantum Computation

2:05 – 2:40 Tai Chiang (University of Illinois, Urbana-Champaign)
Playing with Topological Insulators: Superconductivity and Strain Effects

2:40 – 3:00 Break

Session 4: Identifying Fermionic and Bosonic Topological States (Jessica McChesney)

3:00 – 3:35 Liuyan Zhao (University of Michigan)
Magnetic Excitations in a Honeycomb Ferromagnet

3:35 – 3:35 Mark Dean (Brookhaven National Laboratory)
Observation of Double Weyl Phonons in Parity-breaking FeSi

4:10 – 4:45 Yong P. Chen (Purdue University)
Topological Insulator-based Quantum Devices: From Spin Batteries to Josephson Junctions

4:45 – 5:30 Subramanian Sankaranarayanan (Argonne National Laboratory)
General Discussion

5:30 Adjourn

WK2

Hamiltonian Engineering with Majorana Modes

Ivar Martin[1] and Kartiek Agarwal[2]

[1] Material Science Division, Argonne National Laboratory, Lemont, IL 60439

[2] Department of Physics, McGill University, Montrèal, Quèbec H3A 2T8, Canada

We discuss a new possibility of using braiding operations on Majoranas to engineer novel Hamiltonians. Our proposal is based on the topological robustness of the π phase acquired by Majoranas upon 2π-braiding operations. Repeated application of such braids can be stable to heating if the braiding is performed at high frequencies, by way of pre-thermalization, or by introducing disorder, by way of many-body localization. Repeated braiding can then be used to selectively eliminate certain terms in the Hamiltonian, or enhance others, can be used to engineer additional symmetries and thus realize novel symmetry protected topological phases. The protocol can also be used to stabilize qubits in quantum computers.

Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division.

WK2

Photonic and Bosonic Analogues of Topological Superconductors

Aashish Clerk

Institute of Molecular Engineering, University of Chicago, Chicago, IL 60637

Interest continues to grow in bosonic analogues of topological electronic phases realized using photonic or phononic degrees of freedom. Such devices have a range of potential applications, ranging from new kinds of non-reciprocal devices to sources of entangled photons. Such systems are however typically non-interacting, and have the same band structure and edge state structure as their fermionic counterparts. In this talk, I will discuss recent theory work in my group on a class of bosonic systems where this correspondence fails. They involve using parametric “two-photon” driving, and have Hamiltonians that superficially resemble those of topological superconductors. Among the surprising effects that emerge are the presence of topologically-protected instabilities that can be harnessed for non-reciprocal quantum amplification [1] and squeezing light generation, and effective non-Hermitian dynamics in a bosonic analogue of the Kitaev-Majorana chain [2]. I will discuss

how these ideas could be realized in a variety of different experimental platforms.

[1] V. Peano, M. Houde, F. Marquardt, and A.A. Clerk (2016). *Phys. Rev. X* **6**: 041026.

[2] A. McDonald, T. Pereg-Barnea, and A.A. Clerk (2018). *Phys. Rev. X* **8**: 041031.

WK2

Putative Topological Features in $Co_{1/3}NbS_2$ and Pd_3Pb

J.F. Mitchell[1], Nirmal Ghimire[1], Mojammel Khan[1], Antia Botana[2], and Sam Jiang[1]

[1] Materials Science Division, Argonne National Laboratory, Lemont, IL 60439

[2] Department of Physics, Arizona State University, Tempe, AZ 85281

The recent realization of topological electronic states such as Dirac and Weyl fermions in real materials and their potential for future energy and electronics applications has motivated interest in the study of new forms of topological behavior embodied through new materials. We report here our recent experimental and theoretical work on two such materials, $Co_{1/3}NbS_2$ and Pd_3Pb.

Recently it has been shown that intrinsic part of the anomalous Hall effect (AHE) can be non-zero in non-collinear antiferromagnets as well as in topological materials hosting Weyl nodes near the Fermi energy. We have found a large anomalous Hall effect with Hall conductivity of 30 Ω^{-1} cm^{-1} in a collinear antiferromagnet $Co_{1/3}NbS_2$ with a non-centrosymmetric crystal structure. It orders below 27.5 K with the moments lying in the ab-plane. Magnetization measurement shows the presence of a small ferromagnetic component (0.0013 Bohr magnetons) along c-axis. The large AHE, observed only for H || c, is difficult to reconcile in light of the small ferromagnetic component. Here we will discuss potential alternative explanations of the AHE in $CoNb_3S_6$ framed in terms of topological band structure features or spin texture [1].

Pd_3Pb has been shown theoretically [2] to host unique topological features, including a dispersionless band near the Fermi level and triple nodal points hosting Dirac fermions and open Fermi arcs. Here, we report the crystal growth and electric transport properties of Pd_3Pb. Our low field magnetoresistance measurements indicate an anisotropic Fermi surface. We found that Pd_3Pb manifests a large transverse magnetoresistance, which reaches 650% at 1.8 K and 14 T, and pronounced Shubnikov-de Haas (SdH) oscillations. Preliminary analysis of the field dependence of the SdH oscillations points to the likelihood of nontrivial Berry phase in Pd_3Pb. Preliminary analysis of studies in high field limit will be presented to explore unique features of this unusual fermi surface [3].

Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

[1] N.J. Ghimire et al. (2018). *Nature Communications* **9**: 3280.

[2] K-H Ahn et al. (2018). *Phys. Rev. B* **98**: 035130.

[3] N.J. Ghimire et al. *Phys. Rev. Materials* **2**: 081201.

WK2

Experimental Exploration of Topological Materials

Ni Ni

Physics and Astronomy, University of California, Los Angeles, Los Angeles, CA 90095

New materials are the driving force for technology innovations and our progressive understanding of condensed matter physics. In the last decade, breakthroughs have been made on 3D topological materials. The discovery of bulk materials with non-trivial topology has led to rich new emergent phenomena, including Fermi arc surface state, chiral pumping effect, colossal photovoltaic effect, quantum anomalous Hall effect, etc. In this talk, I will present the exciting progress made in our lab, ranging from the “hydrogen type” topological nodal line semimetal to magnetic topological insulators.

WK2

Tunable Proximity-coupled Topological Superconductor Heterostructures for Quantum Computation

Seongshik Oh

Department of Physics and Astronomy, Rutgers, the State University of New Jersey, Piscataway, NJ 08854

Since the seminal work by Fu and Kane in 2008, heterostructures composed of superconductors (SC) and topological insulators (TI) have been considered a promising platform for producing topological superconductivity (TSC) that can host Majorana particles, the key component for topological quantum computation (TQC). However, despite the relatively well-established theoretical ideas, there has been little progress experimentally and the current prospects to utilize TSC heterostructures for TQC are unclear. The main experimental problems have been the lack of reliable SC/TI materials platforms that have the proper control knobs. Even theoretically, it is only within a small parameter window where the SC/TI heterostructures can lead to the desired TSC phase with Majoranas via a proximity effect in the TI surface states. Therefore, in order to experimentally implement such ideas, it is essential to construct a materials platform where the key materials parameters such as the coupling strength between SC and TI and the Fermi level of TI are under full control. However,

such a materials platform has been so far lacking. Here, I will show that with a series of materials innovations [1–5], we have now come very close to implementing such tunable topological superconductor platforms. With this talk, I would like to open discussion on the prospects and limitations of such tunable topological heterostructures for topological quantum computation.

[1] L. Wu, ..., S. Oh, and N. P. Armitage (2016). "Quantized Faraday and Kerr rotation and axion electrodynamics of the surface states of three-dimensional topological insulators," *Science* **354**: 1124.

[2] M. Salehi, ..., S. Oh (2016). "Finite-Size and Composition-Driven Topological Phase Transition in (Bi1–xInx)2Se3 Thin Films," *Nano Lett.* **16**: 5528.

[3] J. Moon, ..., S. Oh (2018). "Solution to the hole-doping problem and tunable quantum Hall effect in Bi2Se3 thin films," *Nano Lett.* **18**: 820.

[4] P. P. Shibayev, ..., S. Oh (2019). "Engineering topological superlattices and phase diagrams," *Nano Lett.* **19**: 716.

[5] M. Salehi, ..., S. Oh (2019). "Quantum-Hall to insulator transition in ultra-low-carrier-density topological insulator films and a hidden phase of the zeroth Landau level," arXiv:1903.00489.

WK2

Playing with Topological Insulators: Superconductivity and Strain Effects

T.-C. Chiang

University of Illinois at Urbana-Champaign, Urbana, IL 61801

Topological insulators are semiconductors characterized by bulk band gap inversion often caused by strong spin-orbit coupling. By analytic continuation, this gap must close at the surface and reopen outside in vacuum where the gap is noninverted (and infinite). The gap closing at the surface results in metallic surface states, or topological states, which are spin-polarized and span the bulk gap. They carry a surface spin current, largely independent of the details of the surface, which is a feature of strong interest for spintronic applications. This talk will focus on thin films of a prototypical topological insulator Bi_2Se_3 that are (1) made superconducting by proximity coupling to a simple superconducting substrate or (2) strained by stretching a flexible plastic film substrate. Angle-resolved photoemission and x-ray diffraction were employed to determine the electronic structure and the lattice structure. A novel "flip-chip" technique was employed to prepare epitaxial films of Bi_2Se_3 on the superconducting or flexible plastic substrates. We show how the topological surface states are modified under these conditions. Effects of superconducting pairing, coherence, bulk-surface coupling, and electron-lattice coupling will be discussed.

WK2

Magnetic Excitations in a Honeycomb Ferromagnet

Liuyan Zhao

Department of Physics, University of Michigan, Ann Arbor, MI 48109

Two-dimensional (2D) honeycomb ferromagnets are predicted to host massless Dirac magnons because of the two equivalent magnetic sites per unit cell of the honeycomb lattice, mimicking Dirac electrons in graphene. More interestingly, the introduction of the next-nearest-neighbor Dzyaloshinskii-Moriya interaction breaks the sublattice equivalency and suggests the emergence of topological magnons in these honeycomb ferromagnets. In this talk, I will present polarization-resolved Raman spectroscopy studies on magnetic excitations in a honeycomb ferromagnet CrI_3, as a function of temperature, layer number, and magnetic field.

WK2

Observation of Double Weyl Phonons in Parity-breaking FeSi

H. Miao[1], T.T. Zhang[2,3], L. Wang[2,3], D. Meyers[1], A.H. Said[4], Y.L. Wang[1], Y.G. Shi[2], H.M. Weng[2,5], Z. Fang[2,5], and M.P.M. Dean[1]

[1] Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973

[2] Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

[3] University of Chinese Academy of Sciences, Beijing 100049, China

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

[5] Collaborative Innovation Center of Quantum Matter, Beijing 100190, China

Condensed matter systems have now become a fertile ground to discover emerging topological quasiparticles with symmetry protected modes. While many studies have focused on fermionic excitations, the same conceptual framework can also be applied to bosons yielding new types of topological states. Motivated by Zhang et al.'s recent theoretical prediction of double Weyl phonons in transition metal monosilicides [*Phys. Rev. Lett.* **120**: 016401 (2018)], we directly measure the phonon dispersion in parity-breaking FeSi using inelastic x-ray scattering. By comparing the experimental data with theoretical calculations, we make the first observation of double Weyl points in FeSi, which will be an ideal material to explore emerging bosonic excitations and its topologically nontrivial properties [1].

H.M. and M.P.M.D. acknowledge A. Alexandradinata, C. Fang, L. Lu, and D. Mazzone for insightful discussions. This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Early Career Award Program under Award No. 1047478. Work at Brookhaven National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-SC0012704.

The IXS experiments were performed at 30ID in 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 acknowledge the support from the National Key Research and Development Program of China (Grant No. 2016YFA0300600), the National Natural Science Foundation of China (Grants No. 11674369 and No. 11774399), and the Chinese Academy of Sciences (XDB07020100 and QYZDB-SSW-SLH043).

[1] H. Miao et al. (2018). *Phys. Rev. Lett.* **121**: 035302.

WK2
Topological Insulator Based Quantum Devices: From Spin Batteries to Josephson Junctions

Yong P. Chen
Purdue University, West Lafayette, IN 47907

Topological insulators (TI) feature insulating bulk and topologically conducting surfaces with “spin-helical” electrons that may enable a variety of topological quantum information devices. We have demonstrated spin-helical electronic transport [1,2] on the surface of TIs, and further discovered a “topological spin battery effect” [3], opening the possibility to electrically induce and readout a nuclear and electronic spin polarization with exceptionally long lifetime—which we present as a remarkable demonstration of the “topological protection” unique to TI. We further observe unusual behaviors in superconducting Josephson junctions and SQUIDs made out of our Tis [4,5], paving the way for using such spin-helical electrons to realize “topological superconductor” proposed to harbor “majorana fermions” that could enable scalable, topologically-protected quantum computing.

[1] J. Tian et al. (2015). “Electrical injection and detection of spin-polarized currents in topological insulator Bi2Te2Se,” *Sci. Rep.* **5**: 14293.

[2] J. Tian et al. (2019). “On the understanding of current-induced spin polarization of three-dimensional topological insulators,” *Nature Comm.* **10**: 1461.

[3] J. Tian et al. (2017). “Observation of current-induced, long-lived persistent spin polarization in a topological insulator: a rechargeable spin battery,” *Science Advances* **3**: e1602531.

[4] M. Kayyalha et al. (2019). “Anomalous low-temperature enhancement of supercurrent in topological-insulator nanoribbon Josephson junctions: evidence for low-energy Andreev bound states,” *PRL* **122**: 047003.

[5] M. Kayyalha et al. (2019). “Highly skewed current-phase relation in superconductor-topological insulator-superconductor Josephson junctions,” arXiv:1812.00499.

Tuesday, May 7

WK3 APS:
Workshop on Chemical Separations

Location: Building 401, A1100

Time: 8:45 – 5:00

Organizers: Lynne Soderholm (ANL) and Aurora Clark (Washington State)

Chemical-separations researchers represent an untapped user group for synchrotron facilities. X-ray photons offer a variety of opportunities for the chemical separations community, who are struggling with materials performance issues as they look to develop better, more efficient ways to refine natural resources such as petroleum, purify specialty chemicals from rare-earth ores, or deal with effective radioactive-waste disposal. To date researchers in this field have concentrated largely on in-house resources, despite the fact that their problems are on the forefront of some of the most interesting, cutting-edge challenges under study today. For example, most of their materials can be classified as soft matter, including structured solutions, membranes, polymers, and bio-inspired organics. Many systems are amorphous, with hierarchical structuring playing a largely unexplored role in processes of interest.

The opportunity for a mutually beneficial collaboration between chemical-separations researchers and synchrotron-facility personnel lays in answering fundamental questions of structure-function relationships in complex, evolving soft-matter systems. From a separations perspective, synchrotrons can provide information about structuring from local to mesoscopic length scales, providing here-to-fore unavailable insights into the free-energy drivers for these processes. Spectroscopic, scattering, and imaging studies such as those available at the APS would provide new windows into how these separations systems work. The impact of this work is further enhanced when combined with advanced molecular simulations methods that provide a bridge between the molecular level structure and ensemble average measured data. For example, very recent XPCS studies at the APS on the liquid-liquid phase transitions known to impede separations efficacy are resolving questions in favor of a micellar model over a simple biphasic model, thus revealing promising new avenues to resolve this problem. From the APS perspective, SAXS experiments can be used to quantify the structural changes occurring as the phase transition is approached by varying temperature. Dynamics studies reveal aggregate fluctuations on the order of 20 microseconds, just at the limit of current APS capabilities. These studies are informing APS efforts to prepare for the upgrade by providing opportunities to quantify issues ranging from detector-speeds to big-data analysis scenarios.

This workshop will bring together leaders in the fields of separation sciences, modeling and simulation, and machine learning with synchrotron experts in spectroscopy, scattering, and imaging to discuss mutual interests and set the groundwork for collaborative efforts that would benefit all communities involved. Expected outcomes include a roadmap for new ways to integrate these techniques to increase the breadth, applicability, and impact of APS experiments to a diverse and growing chemical-separations user base. Separations is acknowledged as an important impact area within the national research landscape, as demonstrated by the ongoing National Academy of Sciences committee study on A Research Agenda for a New Era of Separations Science.

8:45 – 9:00	Opening Remarks
9:00 – 9:30	Joan Brennecke (The University of Texas at Austin) *Ionic Liquids with Aprotic Heterocyclic Anions for Post-combustion CO_2 Capture*
9:30 – 10:00	Ahmet Uysal (Argonne National Laboratory) *A Necessary Engagement: Surface Science and Chemical Separations*
10:00 – 10:30	David A. Dixon (The University of Alabama) *Predicting the Properties of Actinide Complexes in the Gas Phase and in Solution*
10:30 – 10:45	Break
10:45 – 11:15	Eric Schelter (University of Pennsylvania) *Rare Earth Metals: Challenging Separations and Opportunities for Innovation*
11:15 – 11:45	Uta Ruett (Argonne National Laboratory) *How High-energy X-rays Can Provide Insight into Structure of Liquids*
11:45 – 12:15	Ilan Benjamin (University of California at Santa Cruz) *Surface-active Molecules Influence on Charge Transfer Reactions at Liquid Interfaces*
12:15 – 1:30	Lunch
1:30 – 2:00	Jenifer Shafer (Colorado School of Mines) *Extractant Aggregation in f-element Science: Current Understanding and New Opportunities*
2:00 – 2:30	Mark Antonio (Argonne National Laboratory) *A Telescoping View of Chemical Separations with Synchrotron Radiation*
2:30 – 3:00	David Wu (Colorado School of Mines) *Hierarchical Organization in Associated Structured Phases*
3:00 – 3:15	Break
3:15 – 3:45	Seth Darling (Argonne National Laboratory) *Interface Engineering in Separation Technologies for Water Treatment*
3:45 – 4:15	Michael Servis (Washington State University) *Surfactant-enhanced Heterogeneity of the Aqueous Interface Drives Water Extraction into Organic Solvents*
4:15 – 4:45	Discussion
4:45	Closing Remarks

WK3

Ionic Liquids with Aprotic *Heterocyclic* Anions for Post-combustion CO_2 Capture

Seungmin Oh[1], Tangqiumei Song[2], Gabriela M. Avelar Bonilla[1], Oscar Morales-Collazo[1], and Joan F. Brennecke[1]

[1] McKetta Department of Chemical Engineering, University of Texas at Austin, Austin, TX 78712

[2] Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556

Ionic liquids (ILs) present intriguing possibilities for removal of carbon dioxide from a wide variety of different gas mixtures, including post-combustion flue gas, pre-combustion gases, air, and raw natural gas streams. Even by physical absorption, many ILs provide sufficient selectivity over N_2, O_2, CH_4 and other gases. However, when CO_2 partial pressures are low, the incorporation of functional groups to chemically react with the CO_2 can dramatically increase capacity, while maintaining or even enhancing selectivity. Towards this end, we have developed a series of ionic liquids that include reactive aprotic heterocyclic anions. By incorporating the amine on the anion, they react with CO_2 stoichiometrically (one mole of CO_2 per mole of IL), thus doubling the molar capacity compared to conventional aqueous amine solutions. Moreover, these ILs do not exhibit any viscosity increase upon complexation of the IL with CO_2, because the aprotic heterocyclic anions (AHA ILs) eliminate the pervasive hydrogen bonding and salt bridge formation that is the origin of the viscosity increase.

We have used x-ray scattering to study the structure of these ILs both neat and after reaction with CO_2. Interestingly, the liquid structure is insensitive to the specific anion and whether or not they are reacted with CO_2. We will also describe the discovery of AHA ILs whose melting points when reacted with CO_2 are more than 100°C below the melting point of the unreacted material. These materials allow one to dramatically reduce the energy required for CO_2 release and regeneration of the absorption material because a significant amount of the energy needed for the regeneration comes from the heat of fusion as the material releases CO_2 and turns from liquid to solid. Most recently, we have investigated the effect of encapsulating the AHA ILs in polymeric shells to combat the mass transfer challenges associated with the relatively high viscosity of ILs and show that they maintain their high capacity and can be cycled even in the presence of water.

WK3

A Necessary Engagement: Surface Science and Chemical Separations

Ahmet Uysal

Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

Heavy elements, such as lanthanides and actinides, are very important to modern strategic technologies, including electronics, magnets, and nuclear energy. Therefore, refining and reprocessing of heavy elements in an efficient way is an important challenge, from obtaining the raw materials to handling the waste, during the industrial processes. Solvent extraction, the surfactant-aided preferential transfer of a species from an aqueous to an organic phase, is the most common technique used in heavy and precious metal separations. However, fundamental physical and chemical phenomena behind this process is still not well-understood.

Interfaces play a crucial role in solvent extraction, as the selective adsorption and transfer of ions happen at phase boundaries. Although electrostatics is the major factor determining the interfacial energetics landscape, non-Coulombic weak interactions as well as the interfacial solute and solvent structures are key to selective transfer of similarly charged and sized ions. Therefore, a predictive understanding of interfacial phenomena in heavy element separations require a molecular scale description of all these factors under process conditions, which presents experimental and theoretical challenges. For instance, most empirical and theoretical models of interfacial ion distributions are developed for lighter/smaller ions in low ionic strength solutions. Also, liquid surfaces/interfaces are difficult to access with most structural probes.

We address these challenges by combining state-of-the-art interfacial x-ray scattering and vibrational spectroscopy tools, integrated with molecular dynamics simulations. Interface specific x-ray reflectivity, grazing incidence diffraction, and x-ray fluorescence techniques provide structural information about interfacial ion distributions and ion-extractant structures in the most direct way possible [1]. Sum frequency generation spectroscopy measurements complement the interfacial picture presenting crucial information about interfacial water structures [2]. The molecular dynamics simulations provide a tangible understanding of experimental results [1,2]. With a combination of these methods we acquire a detailed understanding of energetics of ion adsorption at soft interfaces, and structural details of organization and reorganization of metal-amphiphile complexes that drive ion transfer. These studies are naturally integrated with our efforts on chemistry and speciation of heavy ions in aqueous solutions and metal-extractant structures formed in organic solutions.

This work is supported by the U.S. Department of Energy, BES-CSGB, Contract No. DE-AC02-06CH11357. The use of the Advanced Photon Source is also supported by U.S. DOE, BES. ChemMatCARS Sector 15 is supported by the National Science Foundation under grant number NSF/CHE-1346572.

[1] A. Uysal et al. (2017). *J. Phys. Chem. C* **121**(45): 25377–25383.

[2] W. Rock et al. (2018). *J. Phys. Chem. C* **122**(51): 29228–29236.

WK3

Predicting the Properties of Actinide Complexes in the Gas Phase and in Solution

David A. Dixon

Department of Chemistry and Biochemistry, University of Alabama, Tuscaloosa, AL 35487

There is a need to develop new approaches for separations for the actinides for the development of new nuclear reactors for efficient energy generation and for cleaning up the environment at nuclear weapons production sites. In addition, the actinides present a relatively less well-understood domain of chemistry and the presence of *5f* electrons can make the chemistry significantly different from that in other parts of the Periodic Table. Thus, there is substantial interest in understanding the properties and reactivity of molecules containing actinides, including their reactions in aqueous solution. We will describe how computational electronic structure theory can play a role in helping us to understand the actinides and the difficulties in employing such methods for the reliable prediction of the properties of the actinides, for example, the role of relativistic effects. Hydrolysis reactions are important in transformations of actinide ions and oxides into hydroxides. These processes impact environmental transport, nuclear fuel processing, and waste treatment and disposition.

We will describe applications to the hydrolysis chemistry of actinyl dioxide cations AnO_2^+ for An = Pa to Lr, including how their behavior changes with the number of *5f* electrons. The impact of anionic ligands on AnO_2^{2+} will also be discussed. The acidities of aqueous An = Th - Cf in different oxidation states have been calculated with multiple solvation shells and exhibit some interesting trends. These are the first available estimates of the pK_a's for some of these species. Issues in the design of new organic separation agents such as frustrated Lewis basic complexants will be discussed including the potential for separating actinides from lanthanides and issues in the design and synthesis of new complexants, for example solubility.

This work is supported by the U.S. Department of Energy Office of Science (BES) under the Heavy Element and Separations Programs.

WK3

Rare Earth Metals: Challenging Separations and Opportunities for Innovation

Eric J. Schelter

University of Pennsylvania, Philadelphia, PA 19104

The rare earth metals (La-Lu, Sc, and Y) comprise some of the most challenging inter-element separations. Countercurrent solvent extraction is the industry standard for achieving pure materials used applications ranging from permanent magnets to lighting phosphors. These conditions typically operate at or near equilibrium for a single pass extraction or stripping stem, and result in low selectivities. Work in our group has examined different modes of separation. Recently, we initiated a program to examine separations of rare earth metals by kinetic means. We have demonstrated that rate differences for chemical a chemical process tied to rare earth cations can provide means for separation. For example, we have used variable rates of oxidation reactions to partition late rare earth metals. Simple rate equation models also allow for prediction of separations factors. The presentation will highlight recent efforts in this area for the simplified separations of pairs of rare earth species, especially for applications in recycling rare earths from anthropogenic matrices.

WK3

How High-energy X-rays Can Provide Insight into Structure of Liquids

Uta Ruett and Olaf Borkiewicz

Advanced Photon Source, X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439

High-energy x-rays above 50 keV photon energy offer unique possibilities for structural analysis of matter from only locally ordered liquids to long-range ordered single crystals. Systems in complex environments under realistic conditions can be studied because of the high penetration into matter, which is comparable to neutrons.

The Structural Science group at the APS is operating four beamlines with high-energy x-rays. The beamline 11-ID-B is dedicated to the study of nanocrystalline, amorphous and liquid matter and enables collection of total scattering data suitable for pair distribution function (PDF) analysis of wide range of materials. The beamline offers various *in situ* and *operando* capabilities, and can accommodate special sample environments provided by users.

We are continuously developing our capabilities towards multi-modal studies of materials. The station offers a DRIFT spectrometer for certain applications, and allows moderate SAXS measurements providing insights into the shape of particles, information complementary to the PDF. The

future options enabled by the upgrade of the APS will be outlined here.

This presentation will also discuss how the high-energy x-rays can contribute to the understanding of the mechanism of phase separation through structural analysis.

WK3

Surface-active Molecules Influence on Charge Transfer Reactions at Liquid Interfaces

Ilan Benjamin

Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA 95064

Charge transfer reactions such as electron and ion transfer as well as reactions with significant difference in charge distribution between the reactants and products (such as S_N2 and ionization reactions) are very sensitive to the solvent polarity. The dynamics and thermodynamics of these reactions are strongly influenced by the heterogeneous character of the liquid/liquid and liquid/vapor interfaces where the polarity of the media changes rapidly over a sub-nanometer length scale and by surface density fluctuations. Surface-active molecules that are adsorbed at the interface and interacts with the reactants can provide a local reaction environment whose polarity is further distinguished from that of the neat interface. We examine how these surface-active molecules affect reactivity and how their effect is influenced by the local structure and dynamics of the interface.

WK3

Extractant Aggregation in F-element Science: Current Understanding and New Opportunities

M.J. Servis[1], A.G. Baldwin[1], D. Wu[1], A. Clark[2], and J.C. Shafer[1]

[1] Department of Chemistry, Colorado School of Mines, Golden, CO 80401

[2] Department Chemistry, Washington State University, Pullman, WA 99163

Supramolecular assembly has been integral to the management of used nuclear fuel since the initial, ether-based solvent extraction process used to purify uranium and attempted during the Manhattan project. Solvating extractants, which rely on supramolecular assembly, are an ideal partner for purifying the *f*-elements away from the rest of the periodic table. The general mechanism for metal recovery by a solvating reagent includes the interaction of a charge neutral, strong dipole amphiphile and charge balancing counter ions with a metal center to solubilize this metal center into the organic phase. This general mechanism is well depicted by a coordination chemistry model, where the metal sits in the center of the coordination complex and the amphiphile and counter-ions populate the metal coordination sphere, however this mechanism probably underestimates the importance of hydrogen bonding and other ion-dipole interactions that control intermediate (second and third coordination shell) and long (bulk material) range interactions. These interactions can control other important phenomena, such as third phase formation, and the combination of x-ray scattering techniques and molecular dynamics simulation is proving to be a powerful partnership in providing molecular level resolution with experimentally determined measurables. This presentation will be an overview of recent findings from this research group, as well as a review of the broader literature pertaining to solvating extractants and extractant aggregation, to highlight the opportunities for using beamline techniques to examine extraction mechanisms most relevant to *f*-element science.

WK3

A Telescoping View of Chemical Separations with Synchrotron Radiation

Mark R. Antonio

Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

The advent of intense, tunable- and scanable-wavelength x-rays has revolutionized many disciplines in physical sciences and engineering. Although the separation science communities have been slow to embrace the myriad characterization capabilities available at synchrotron user facilities, it is not hyperbole to state that synchrotron x-radiation is advancing the field of chemical separations in ways that would be difficult, if not impossible, to realize with conventional tube sources. For example, in applications related to equilibrium separations based on differences in solute transfer across liquid-liquid and liquid-gas phase boundaries, the techniques of x-ray absorption spectroscopy and small-angle x-ray scattering are opening new vistas of understanding with unprecedented sensitivity and resolution. Examples from the literature of liquid-liquid extraction will be discussed to benchmark the role that synchrotron research plays in unraveling wickedly complex, fundamental issues in the profusion of separation methods used in industrial- and bench-scale process chemistry. The way forward includes the use of the full armamentarium of synchrotron instrumentation and techniques—scattering, spectroscopy, and imaging alike—to provide a transformative, telescoping view of separation science on interconnected length-, time-, and energy-scales. A multimodal, multiscale approach towards characterization of separations processes will provide a unified view of targeted solutes in equilibrium phases and at phase boundaries,

thereby enabling deliberate and rational design of high-performance systems by tailoring mass transfer processes in a hierarchical fashion in both space and time.

This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Biosciences and Geosciences, under Contract No. DE-AC02-06CH11357.

WK3
Hierarchical Organization in Associated Structured Phases

David T. Wu
Department of Chemistry and Department of Chemical and Biological Engineering, Colorado School of Mines, Golden, CO 80401

Chemical separations involve the partitioning of molecules according to differences in interactions, such as hydrophobic, hydrogen bonding, charge, polar, steric and ligand complexation interactions. From a condensed matter perspective, balance and frustration between such competing interactions, such as those that exist in amphiphilic surfactant systems or analogous frustrated magnetic systems, can lead to rich structured phases. Moreover, this competition at the molecular level often leads to structure at greater length scales, for instance, the formation of micelles or other extended mesophases that emerge from the association of surfactant molecules. The characterization and understanding of this higher-order structure can be relevant for chemical separation processes.

In this talk, I will present an overview of systems we have studied exhibiting such hierarchical organization:

- Cooperative association of methane and water molecules in controlling the nucleation of clathrate hydrate lattices
- Electric-field directed assembly of anisotropic colloids into complex phases
- Virus capsid protein assembly: autocatalysis and error-correction
- Association and aggregation of extractant/water/acid molecules into hydrogen-bonded networks in solvent extraction systems

I will highlight our use of simulation and theory, in close connection with experiment when possible, to understand both equilibrium and kinetic properties of these systems.

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[2] F. Ma, D.T. Wu, and N. Wu (2013). "Formation of Colloidal Molecules Induced by Alternating-Current Electric Fields," *J. Am. Chem. Soc.* **135**: 7839–7842.

[3] F.D. Ma, S.J. Wang, D.T. Wu, and N. Wu (2015). "Electric-field-induced assembly and propulsion of chiral colloidal clusters," *P. Natl. Acad. Sci. USA* **112**: 6307–6312.

[4] G.L. Casini, D. Graham, D. Heine, R.L. Garcea, and D.T. Wu (2004). "*In vitro* papillomavirus capsid assembly analyzed by light scattering," *Virology* **325**: 320–327.

[5] M.J. Servis, D.T. Wu, and J.C. Braley (2017). "Network analysis and percolation transition in hydrogen bonded clusters: nitric acid and water extracted by tributyl phosphate," *Phys. Chem. Chem. Phys.* **19**: 11326–11339.

[6] M.J. Servis, D.T. Wu, J.C. Shafer, and A.E. Clark (2018). "Square supramolecular assemblies of uranyl complexes in organic solvents," *Chem. Commun. (Camb)* **54**: 10064–10067.

WK3
Interface Engineering in Separation Technologies for Water Treatment

Seth B. Darling
Institute for Molecular Engineering, Argonne National Laboratory, Lemont, IL 60439

Advanced Materials for Energy-Water Systems EFRC, Argonne National Laboratory, Lemont, IL 60439

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Institute for Molecular Engineering, University of Chicago, Chicago, IL 60615

Driven by climate change, population growth, development, urbanization, and other factors, water crises represent the greatest global risk in the coming decades. Advances in materials represent a powerful tool to address many of these challenges. Understanding—and ultimately controlling—interfaces between materials and water are pivotal [1]. In this presentation, Dr. Darling will lay out the challenges and present several examples of work in his group based on materials science strategies for addressing applications in water. In each instance, manipulation of interfacial properties provides novel functionality, ranging from selective transport to energy transduction to pollution mitigation.

This work was supported as part of the Advanced Materials for Energy-Water Systems (AMEWS) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department

of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

[1] *J. Appl. Phys.* **124**: 030901 (2018).

WK3

Surfactant-enhanced Heterogeneity of the Aqueous Interface Drives Water Extraction into Organic Solvents

Michael J. Servis[1] and Aurora E. Clark[1,2]

[1] Department of Chemistry, Washington State University, Pullman, WA 99163

[2]Pacific Northwest National Laboratory, Richland, WA 99352

Liquid/liquid interfaces are essential to certain chemical separations processes, such as solvent extraction. In solvent extraction, an amphiphilic extractant molecule forms complexes with aqueous-soluble molecules at the liquid/liquid interface to extract those aqueous molecules into an organic solvent. Despite the importance of those complexation reactions on the underlying kinetics of solvent extraction, understanding of the molecular structure at the interface is lacking in large part due to the challenges associated with probing the interfacial environment with experimental approaches such as x-ray reflectivity. Many of those challenges stem from molecular-scale thermal fluctuations of the interface, which impart structural heterogeneity across the aqueous surface. That heterogeneity is further enhanced by the presence of the surface-active extractant molecules.

Here, molecular dynamics simulations are applied to investigate the structural characteristics of the water/extractant hydrogen bonded network at the interface in response to extractant adsorption. Additionally, a mechanism by which the extractant transports water from the aqueous interface into the organic phase is identified. A graph theory topological analysis method is developed to quantify the role of hydrogen bonded clusters of water and extractant protruding from the aqueous surface in the water transport process. The chemical insight and analysis methodology presented here may be broadly applied to study molecular structure and reactions at surfactant-laden liquid/liquid interfaces and assist in interpretation of experimental data.

Tuesday, May 7

WK4 CNM:
Photon Qubit Entanglement and Transduction

Location: Building 401, Room A5000

Time: 8:30 – 5:00

Organizers: Xuedan Ma, Xufeng Zhang, and Stephen Gray (all CNM)

Various quantum systems that are suitable for specific applications have been developed in the past few years based on a broad range of physical platforms. To further exploit the advantages of quantum technology for complicated tasks in computation, communication, and sensing, it has becoming increasingly pressing to develop distributed quantum networks that combine the advantages of different quantum systems. Such distributed quantum networks require the development of individual quantum systems that operate in both the microwave and optical domains, as well as high fidelity transductions among different systems to interconnect quantum information of different formats. Despite of the fast development in microwave qubits based on superconducting technologies, deterministic optical single-photon sources and the related optical photonic components are still underdeveloped, which, as a result, hinders the development of long-distance quantum links. On the other hand, high-efficiency quantum interconnections between superconducting and optical systems are also missing because of the intrinsic incompatibility of the superconducting technique with optical photons and their huge frequency difference, which pose a significant challenge in encoding/decoding the microwave quantum information to the optical quantum link.

In this workshop, we aim to bring together researchers working on various aspects of photon qubits and quantum transduction systems to discuss pathways towards addressing these grand challenges faced by the quantum network community. This is a highly interdisciplinary research topic that involves efforts from a broad community including quantum optics, superconducting qubits, optomechanics. Effective communication among researchers of different backgrounds will greatly help to explore novel opportunities for designing and implementing photon qubit entanglement and transduction. It will also help create synergies between Argonne/CNM and the worldwide scientific community. With CNM's efforts towards developing a high standard user facility to support the increasing need for quantum infrastructure, this workshop will be a great opportunity for outreaching to potential users and obtaining valuable feedbacks.

Main topics in this workshop include:

- Quantum photonic materials and devices
- Novel quantum transduction approaches and material systems
- Photonic quantum networks and links
- Quantum repeaters and memories

Session 1: Quantum Optics and Nanophotonics (Session Chair: Xuedan Ma)

8:30 – 9:15 Qiang Lin (University of Rochester)
Manipulating Quantum States of Photons on Integrated Photonic Chips

9:15 – 10:00 Virginia Lorenz (University of Illinois, Urbana-Champaign)
Engineering Photonic Quantum States for Quantum Applications

10:00 – 10:30 Break

10:30 – 11:15 Michael Reimer (University of Waterloo)
On-demand Generation of Bright Entangled Photon Pairs

11:15 – 12:00 German Kolmakov (NYC College of Technology, CUNY)
Optical Detection and Storage of Entanglement in Plasmonically Coupled Quantum-dot Qubits

12:00 – 1:30 Lunch

1:30 – 2:15 Nick Vamivakas (University of Rochester)
Quantum Optics with Atomically Thin Materials

Session 2: Quantum Transduction Systems (Session Chair: Xufeng Zhang)

2:15 – 3:00 Hailin Wang (University of Oregon)
Mechanically Mediated Quantum Networks of Spins in Diamond

3:00 – 3:30 Break

3:30 – 4:15 Hoi-Kwan Lau (The University of Chicago)
High-fidelity Bosonic Quantum State Transfer Using Imperfect Transducers and Interference

4:15 – 5:00 Miguel Levy (Michigan Technological University)
Faraday Effect Enhancement in Nanoscale Iron Garnet Films

5:00 Adjourn

WK4

Manipulating Quantum States of Photons on Integrated Photonic Chips

Qiang Lin
Department of Electrical and Computer Engineering, University of Rochester, Rochester, NY 14627

Recent advances in quantum photonics have resulted in broad applications ranging from secure communication, metrology, sensing, to advanced computing. Chip-scale implementation would not only enhance the complexity and capacity of information processing, but also enable novel functionalities, which are otherwise inaccessible in room-wide/table-top experiments.

Lying in the heart of these applications is the capability of generating and manipulating versatile high-purity entangled photonic quantum states. In this talk, we will discuss our recent effort in engineering micro/nanophotonic device structures for producing and manipulating photonic quantum states on various chip-scale device platforms, by taking advantage of enhanced four-wave mixing and parametric down conversion processes, via the second-order and third-order optical nonlinearities.

WK4

Engineering Photonic Quantum States for Quantum Applications

Virginia O. Lorenz
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801

Photonic quantum states are good carriers of quantum information because they are robust to environmental fluctuations, but generating photons with just the right properties for specific applications is still a challenge. I will present our work on generating, engineering and characterizing photonic quantum states for quantum applications, including our demonstrations of novel photon-pair sources, bi- and tri-partite entangled states, and efficient characterization techniques.

WK4

On-demand Generation of Bright Entangled Photon Pairs

M.E. Reimer

Institute for Quantum Computing, and Department of Electrical and Computer Engineering, University of Waterloo, Waterloo, ON N2L 3G1, Canada

The on-demand generation of bright entangled photon pairs is an essential resource in quantum optics, quantum communication and quantum sensing. However, a bright entangled photon source with near-unity fidelity and efficiency is currently lacking. In this talk, I will present the generation of dephasing-free entangled photon pairs from a nanowire quantum dot with high brightness and collection efficiency [1]. We prove through our research that it is possible to reach perfect entanglement fidelity with current technology by also considering the detection process *in addition to* the generation process, even in an indium rich quantum dot with a large nuclear spin.

Finally, I will present two approaches to reach the perfect entangled photon source with near-unity fidelity and efficiency. These two approaches rely on the need to remove the fine structure splitting of the intermediate exciton states in the biexciton-exciton cascade as a finite fine structure splitting has been shown to degrade the entanglement fidelity. First, I will discuss our novel gating strategy with a quadrupole electrostatic potential, which shows that the fine structure splitting can be erased for any quantum dot dipole orientation without comprising the quantum dot brightness [2]. Second, I will present our all-optical approach to compensate the fine structure splitting by employing a fast rotating waveplate emulated by a high frequency shifter [3]. This latter approach has the unique advantage that the fine structure splitting of quantum dots in photonic nanostructures such as nanowires and micropillars can be directly compensated for without the need for further sample processing.

In this presentation, I will discuss these two important points: dephasing free entangled photons and no fine structure splitting, both of which lead us further towards the perfect source of entangled photons. With this work, we make great strides forward to transition out of the lab into practical and powerful real-world applications, such as information security for the day-to-day user as well as quantum radar which positively influences strategies of national defence.

[1] A. Fognini et al. (2017). "Path to perfect photon entanglement with a quantum dot," arXiv:1710.10815.

[2] M. Zeeshan et al. (2018). "Quadrupole electric field for erasing the fine structure splitting in a single quantum dot," arXiv:1809.02538.

[3] A. Fognini et al. (2018). "Universal fine-structure eraser for quantum dots," *Opt. Express* **26**: 24487–24496.

WK4

Optical Detection and Storage of Entanglement in Plasmonically Coupled Quantum-dot Qubits

Matthew Otten[1], Stephen K. Gray[1], and German V. Kolmakov[2]

[1] Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439

[2] Physics Department, New York City College of Technology, City University of New York, Brooklyn, NY 11201

Recent proposals and advances in quantum simulations, quantum cryptography, and quantum communications substantially rely on quantum entanglement formation. Contrary to the conventional wisdom that dissipation destroys quantum coherence, coupling with a dissipative environment can also generate entanglement. We consider a system composed of two quantum-dot qubits coupled with a common, damped surface plasmon mode; each quantum dot is also coupled to a separate photonic cavity mode. Cavity quantum electrodynamics calculations [1] show that upon optical excitation by a femtosecond laser pulse, entanglement of the quantum-dot excitons occurs, and the time evolution of the $g^{(2)}$ pair correlation function of the cavity photons is an indicator of the entanglement. We also show that the degree of entanglement is conserved during the time evolution of the system. Furthermore, if coupling of the photonic cavity and quantum-dot modes is large enough, the quantum-dot entanglement can be transferred to the cavity modes to increase the overall entanglement lifetime. This latter phenomenon can be viewed as a signature of entangled, long-lived quantum-dot exciton-polariton formation. The preservation of total entanglement in the strong-coupling limit of the cavity–quantum-dot interactions suggests a novel means of entanglement storage and manipulation in high-quality optical cavities

The authors thank Xuedan Ma for helpful discussions. G.V.K. gratefully acknowledges support from the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Visiting Faculty Program (VFP). G.V.K. is also grateful to the U.S. Department of Defense for partial support under Contract No. W911NF1810433. This work was performed, in part, at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

[1] M. Otten, S.K. Gray, and G.V. Kolmakov (2019). "Optical detection and storage of entanglement in plasmonically coupled quantum-dot qubits," *Physical Review A* **99**(3): 032339.

WK4

Quantum Optics with Atomically Thin Materials

A. Nick Vamivakas

The Institute of Optics, University of Rochester, Rochester, NY 14627

Department of Physics, University of Rochester, Rochester, NY 14627

Center for Coherence and Quantum Optics, University of Rochester, Rochester, NY 14627

Two-dimensional, atomically-thin, materials have received enormous interest as a result of their unique mechanical, electrical and optical properties. Particularly exciting are the transition metal dichalcogenides—atomically-thin semiconductors that possess an electronic band gap in the visible. Although these materials have been investigated for applications in opto-electronics, not much work has focused on these systems as a platform for quantum photonics and quantum optics.

In this talk, I will describe two approaches that leverage atomically thin semiconductors, and other two-dimensional materials, assembled in layered van der Waals heterostructures for applications in these areas. In the first part of the talk, I will describe the unique photophysical properties of quantum emitters hosted by single layer transition metal dichalcogenides. I will describe our recent efforts to control the confined excitons and subsequent single photon generation. Finally, I will report on the observation of the coherent evolution of quantum emitters in the insulator hexagonal boron nitride.

WK4

Mechanically-mediated Quantum Networks of Spins in Diamond

Hailin Wang

Department of Physics, University of Oregon, Eugene, OR 97403

Phonons, which are the quanta of mechanical waves, are immune to scattering loss into vacuum and can couple to a variety of quantum systems. These distinct properties can enable new experimental platforms for quantum computing and quantum communication. In this talk, I will discuss the design and experimental implementation of a phononic quantum network of spins, in which individual spin qubits in diamond couple to a network of nanomechanical oscillators. I will also consider a spin-photon interface that explores quantum transduction between spins and photons through their coupling to a common mechanical oscillator. These mechanically-mediated networks can overcome or circumvent many of the inherent difficulties of direct optical networks of spins qubits.

WK4

High-fidelity Bosonic Quantum State Transfer Using Imperfect Transducers and Interference

Hoi-Kwan Lau and Aashish A. Clerk

Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637

We consider imperfect two-mode bosonic quantum transducers that cannot completely transfer an initial source-system quantum state due to insufficient coupling strength or other Hamiltonian non-idealities. We show that such transducers can generically be made perfect by using interference and phase-sensitive amplification. Our approach is based on the realization that a particular kind of imperfect transducer (one which implements a swapped quantum non-demolition (QND) gate) can be made into a perfect one-way transducer using feed-forward and/or injected squeezing. We show that a generic imperfect transducer can be reduced to this case by repeating the imperfect transduction operation twice, interspersed with amplification. Crucially, our scheme only requires the ability to implement squeezing operations and/or homodyne measurement on one of the two modes involved. It is thus ideally suited to schemes where there is an asymmetry in the ability to control the two coupled systems (e.g., -to-optics quantum state transfer). We also discuss a correction protocol that requires no injected squeezing and/or feed-forward operation.

Hoi-Kwan Lau and Aashish A. Clerk (2019).
npj Quantum Information **5**: 31.

WK4

Faraday Effect Enhancement in Nanoscale Iron Garnet Films

Miguel Levy[1], Olga Borovkova[2], and Vladimir Belotelov[2]

[1] Michigan Technological University, Physics Department, Houghton, MI 49931

[2] Russian Quantum Center, Moscow, Russia

This presentation reports on a newly discovered enhancement mechanism of the magneto-optic Faraday Effect in nanoscale bismuth-substituted iron garnet films. Iron garnets are widely used in the fabrication of optical isolators, circulators and modulators because of the nonreciprocal nature of this effect.

In the last quarter of the 20th century, elemental substitutions were found to enhance the nonreciprocal response of these systems, and advances in isolator device on-chip integration made extensive used of this technology, especially for telecom applications. However, no further elemental substitutions have been found to yield comparable improvement in recent decades. Other

approaches such as photonic-crystal and ring resonator techniques were developed since, but at the expense of optical bandwidth. Present day industrial need for nanoscale nonreciprocal photonic on-chip and broad band devices in the telecom regime thus call for further advances in magneto-optical functional strength.

The work we present in this talk reports on an as yet untapped approach to nonreciprocal functional magnification. The methodology does not rely on resonant effects or elemental substitution mechanisms, but rather on symmetry-breaking at the surface. A seven-fold magnification of the magneto-optic gyrotropy parameter responsible for the Faraday Effect is observed, occurring within a few monolayers of the iron garnet crystal surface. Rigorous electromagnetic calculations show that classical theory cannot account for the observe phenomena, pointing to fundamental departures from the classical magneto-optic response.

Wednesday, May 8

WK5 APS:
RIXS after the APS Upgrade: Science Opportunities

Location: Building 402, Room E1100/1200

Time: 8:30 – 5:00 followed by a one-hour beamline tour

Organizers: Diego Casa and Jungho Kim (Argonne National Laboratory)

For resonant inelastic x-ray scattering (RIXS) at beamline 27-ID, the APS upgrade offers unprecedented opportunities for enhancements of the technique and the beamline, which will greatly benefit users of the facility. The vastly increased brightness of the x-ray source and a higher overall flux will enable ultra-high-resolution measurements (<10meV) that are not feasible today. These experiments will require both smaller focal spot sizes (<5um) and tighter incident energy bandpasses (<10meV).

A novel prototype RIXS flat-crystal spectrometer was recently implemented at beamline 27-ID at the Advanced Photon Source in anticipation of the upgraded source. It established a new record resolution for RIXS below 10 meV, together with a promise to do even better soon. To fully harness the benefits of such a vastly improved source and optics, parallel improvements to beamline instrumentation will include a more precise (<10um sphere-of-confusion) and efficient spectrometer, a more flexible high-resolution tunable monochromator with selectable bandpass down to ~5meV, and crucially practical implementations of meaningful in situ sample environments, including high-pressure and strong magnetic fields.

The aim of this workshop is to bring together the RIXS community to chart the roadmap ahead, considering how the technical upgrades can enable advances on the many exciting scientific opportunities from materials science from both practical and fundamental perspectives. In addition to presentations from our user community on forefront RIXS science, a review of RIXS experimental considerations and design, along with RIXS data simulation, numerical methods and analysis will be offered, culminating in an open session and a beamline tour.

8:30 – 8:40 Thomas Gog (Argonne National Laboratory)
Opening Remarks

8:40 – 9:20 Jeroen van den Brink (Institute for Theoretical Solid State Physics, IFW Dresden)
Resonant Inelastic X-ray Scattering on High-Tc Cuprates and Magnetic Iridates

9:20 – 10:00 Michel van Veenendaal (Northern Illinois University)
Non-equilbrium X-ray Spectroscopy in Fe-Co Prussian Blue Analogue Spin-crossover Complex

10:00 – 10:30 Break

10:30 – 11:00 Gábor B. Halász (Oak Ridge National Laboratory)
Probing Quantum Spin Liquids with Resonant Inelastic X-ray scattering

11:00 – 11:30 Yilin Wang (Brookhaven National Laboratory)
EDRIXS: An Open Source Toolkit for Simulating Spectra of Resonant Inelastic X-ray Scattering

11:30 – 12:00 Diego Casa and Ayman Said (Argonne National Laboratory)
Proposed RIXS Instrumentation

12:00 – 1:30 Lunch

1:30 – 2:00 Jason Hancock (University of Connecticut)
Local and Itinerant Electronic Structure in Rare-earth Intermetallics

2:00 – 2:30 Alex Frano (University of California, San Diego)
RIXS with In Situ *Magnetic Field: Towards Understanding the Complex Magnetism of Li_2IrO_3*

2:30 – 3:00 Gilberto Fernandes Lopes Fabbris (Argonne National Laboratory)
RIXS at High Pressure: Challenges and Opportunities

3:00 – 3:30 Break

3:30 – 4:00 Wentao Jin (University of Toronto)
RIXS Study of Sr_2IrO_4 Single Crystal under Uniaxial Strain

4:00 – 4:30 Ryan Hadt (California Institute of Technology)
Applications of Resonant X-ray Emission and Inelastic X-ray Scattering in Chemistry and Biology

4:30 – 4:55 Jungho Kim (Argonne National Laboratory)
Open session

4:55 – 5:00 Thomas Gog (Argonne National Laboratory)
Wrap-up

5:00 Mary Upton (Argonne National Laboratory)
27-ID RIXS Beamline tour

WK5

Resonant Inelastic X-ray Scattering on High-Tc Cuprates and Magnetic Iridates

Jeroen van den Brink
Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden Helmholtzstraße 20, 01069 Dresden, Germany

Department of Physics, Washington University, St. Louis, MO 63130

Resonant inelastic x-ray scattering (RIXS) provides direct access to elementary charge, spin and orbital excitations in complex oxides. As a technique, it has made tremendous progress with the advent high-brilliance synchrotron x-ray sources. From the theoretical perspective, a fundamental question is to precisely which low-energy correlation functions RIXS is sensitive. Depending on the experimental RIXS setup, the measured charge dynamics can include charge-transfer, phonon, d-d, and orbital excitations. The focus of this talk will be on RIXS as a probe of spin dynamics and the electron-phonon coupling in high-Tc cuprates and the combined magnetic and orbital modes in strongly spin-orbit coupled iridium-oxides.

WK5

Nonequilbrium X-ray Spectroscopy in Fe-Co Prussian Blue Analogue Spin-crossover Complex

M. van Veenendaal
Northern Illinois University, DeKalb, IL 60115

Nonequilibrium x-ray spectroscopy is studied for a model spin crossover compound. The ultrafast spincrossover is calculated for Fe-Co Prussian blue analogues using a dissipative quantum-mechanical model of a cobalt ion coupled to a breathing mode [1,2]. All electronic interactions are treated on an equal footing. The divalent cobalt ion reaches 90% of the $S = 3/2$ value within 20 fs after photoexciting a low-spin Co^{3+} ion by an iron-to-cobalt charge transfer. The doublet-to-quartet spin crossover is significantly faster than the oscillation period of the breathing mode. The system relaxes to the lowest manifold of divalent cobalt ($^4T_1$) in 150–200 fs. Resonant inelastic x-ray scattering and x-ray absorption are calculated from the time-dependent nonequilibrium wavefunction. The resulting spectra cannot be decomposed into incoherent superpositions of transient states. Oscillations in the spin-orbit coupling gives rise to strong variations in the isotropic branching ratio. The RIXS shows crystal field oscillations and strong anti-Stokes effects.

[1] M. van Veenendaal (2017). *Scientific Reports* **7**: 6672.

[2] M. van Veenendaal (2018). *Phys. Rev. B* **97**: 125108.

WK5

Probing Quantum Spin Liquids with Resonant Inelastic X-ray Scattering

Gábor B. Halász

Oak Ridge National Laboratory, Oak Ridge, TN 37830

It is difficult to identify quantum spin liquids in experimental candidate materials due to the lack of direct "smoking gun" signatures. We propose that resonant inelastic x-ray scattering (RIXS) is an effective probe to detect spin-liquid physics in potential material incarnations of the Kitaev spin liquid (such as the honeycomb iridates and α-$RuCl_3$). Different RIXS channels pick up the fractionalized excitations of the Kitaev spin liquid separately and, in particular, the non-spin-flip channel can probe the characteristic momentum dispersion of the gapless Majorana excitations. As a signature of symmetry fractionalization, the corresponding RIXS response is suppressed around the Γ point of the Brillouin zone.

WK5

EDRIXS: An Open Source Toolkit for Simulating Spectra of Resonant Inelastic X-ray Scattering

Y.L. Wang[1], G. Fabbris[1], M.P.M. Dean[1], and G. Kotliar[1,2]

[1] Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, Upton, NY 11973

[2] Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08856

In this talk, we present an open source toolkit (dubbed EDRIXS) [1] to facilitate the simulations of RIXS spectra of strongly correlated materials based on exact diagonalization (ED) of certain model Hamiltonians. The model Hamiltonian can be from a single atom, small cluster or Anderson impurity model, with model parameters from density functional theory plus Wannier90 or dynamical mean-field theory calculations. The spectra of x-ray absorption spectroscopy (XAS) and RIXS are then calculated using Krylov subspace techniques. This toolkit contains highly efficient ED, XAS and RIXS solvers written in modern Fortran 90 language and a convenient Python library used to prepare inputs and set up calculations. We first give a short introduction to RIXS spectroscopy, and then we discuss the implementation details of this toolkit. Finally, we show several examples [2] to demonstrate its usage.

[1] Y.L. Wang, G. Fabbris, M.P.M. Dean, and G. Kotliar, arXiv:1812.05735.

[2] Y.L. Wang, Ruitang Wang, Jungho Kim, M.H. Upton, D. Casa, T. Gog, G. Cao, G. Kotliar, M.P.M. Dean, and X. Liu, arXiv:1810.05243. Accepted by PRL.

WK5

Local and Itinerant Electronic Structure in Rare-earth Intermetallics

Jason N. Hancock[1], Donal Sheets[1], Maxim Dzero[2], Daniel Mazzone[3], and Ignace Jarrige[3]

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Rare earth materials represent the ultimate limit of electronic correlations and present a rich landscape for exploring phenomena in electron-correlated and topological quantum matter. Central to the physics of these materials is the admixture of strongly correlated and localized magnetic degrees of freedom with itinerant states across the electronic bandwidth. Resonant spectroscopies like resonant inelastic x-ray scattering present unique opportunities to control and direct interrogation of quantum wavefunctions between the local and itinerant limits. In this talk, we will show how progress in this direction has been evolving over the past decade with strong support from synchrotron endstation improvements at the APS and around the world. In particular, we will show results at the rare-earth *L* edges crossing the valence transitions in $YbInCu_4$ and $Sm_{1-x}Y_xS$, with complementary work at the soft x-ray *M* edges of these and related materials. Together, these science-driven benchmarks in discovery make a strong and compelling case to support upgrades such as the APS-U project and show the synergy between the user community and pioneers of instrumentation at the APS can strengthen old and usher new activity areas in science.

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WK5

RIXS with *in situ* Magnetic Field: Towards Understanding the Complex Magnetism of Li_2IrO_3

Alejandro Ruiz[1], Anthony Allen[1], Vikram Nagarajan[2], Isaac Zinda[3], Jake Koralek[4], Mary Upton[5], Jungho Kim[5], Nicholas Breznay[3], James Analytis[2], Diego Casa[5], and Alex Frañó[1]

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Unconventional magnetism appears in correlated electron systems with strong spin-orbit coupling. 5d iridate compounds coordinated in a honeycomb lattice like Li_2IrO_3 are a promising avenue to realize the peculiar anisotropic, frustrated magnetism scenario of Kitaev's Hamiltonian [1,2] which could host a quantum spin liquid ground state. Experimentally, the material displays a degeneracy of magnetic ground states upon the application of a magnetic field [3]: one incommensurate spiral and a commensurate 'zigzag' phase. The mechanism by which the magnetic order and the associated low-energy excitations vary with magnetic field is unknown. Measuring the excitation spectrum associated with each of the two magnetic phases is challenging for two reasons: the energy scale of said excitations is low and thus at the limit of experimental resolution of RIXS spectrometers, and the application of in-situ magnetic fields within RIXS chambers is highly challenging.

Using the state-of-the-art RIXS spectrometer at Sector 27 of the Advanced Photon Source, we have overcome both challenges to measure the spin excitations of both spiral and commensurate phases by tracking low-energy excitations near their respective q-vectors in an applied magnetic field of 2 Tesla (as well as 0 Tesla). We have identified magnon branches near each q-vector.

Surprisingly, the magnon velocity near the spiral q-vector is much higher than the expected *sin(qa/2)* behavior, possibly suggesting a larger magnetic coupling strength than previously thought. This data may provide insight into the interactions between pseudo-spins in this fascinating material. Finally, we will discuss how the application of modest magnetic fields within modern high-resolution RIXS setups is now possible and will open up interesting new avenues of research in exotic 5d-magnetism.

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.

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WK5

RIXS at High Pressure: Challenges and Opportunities

Gilberto Fabbris

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Pressure is a key thermodynamic variable that can be used not only to understand material properties, but also to drive novel phenomena. However, high-pressure techniques often impose strict experimental constraints, which drastically limits the pressure range available for certain techniques. This is particularly problematic for magnetic and electronic properties, for which, despite recent advances, probes such as inelastic neutron scattering and magnetometry are often restricted to pressures below 10 GPa. Over the last decade, RIXS has emerged as a key material science technique due to its ability to probe various types of magnetic, electronic and lattice excitations, making its implementation in the high-pressure regime highly desirable [1]. In this talk, I will focus on the technical challenges of probing RIXS at high-pressure. This will be done with the aid of two scientific examples: the nature of Sr_2IrO_4 high-pressure quantum paramagnetism [2], and the interplay between Cu 3d and Ir 5d orbitals in Cu_2IrO_3 [3]. I will also discuss potential instrument developments and the impact of APS-U on high-pressure RIXS experiments.

Work at Argonne is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC-02-06CH11357.

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WK5

RIXS Study of Sr_2IrO_4 Single Crystal under Uniaxial Strain

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It has been shown that the structural details, such as the Ir-O-Ir angle and the Ir-Ir distance, play an important role in influencing the magnetic properties of spin-orbital entangled iridates. But it is not well understood how the electronic structure and magnetic interaction in the iridates respond to structural distortion. The application of uniaxial strain within the *ab* plane can break tetragonal symmetry and induce the lattice distortion. In addition, the distortion can be continuously tuned, allowing one to examine the pseudospin-lattice coupling. Using our homemade piezoelectric-based strain apparatus, we have performed Ir L_3-edge RIXS measurements on single-crystal Sr_2IrO_4 under uniaxial tensile/compressive strain applied along the in-plane (1 0 0) and (1 1 0) directions. In both cases, we are able to drive the lattice distortion to the magnitude of 10^{-3} and tune the magnetic domain structure in Sr_2IrO_4 accordingly, while the change in the magnetic excitation is found to be quite marginal within this level of distortion. This indicates that the in-plane magnon gap in Sr_2IrO_4 is relatively robust with respect to the uniaxial perturbation, and a larger magnitude of orthorhombic distortion than 10^{-3} is needed to induce the gap change.

WK5

Applications of Resonant X-ray Emission and Inelastic X-ray Scattering in Chemistry and Biology

Ryan G. Hadt

Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125

Transition metal electronic structure plays important roles across chemistry, biology, and physics. This presentation will discuss recent applications of resonant x-ray emission spectroscopy (RXES) and resonant inelastic x-ray scattering (RIXS) in defining the roles of transition metals in bioinorganic chemistry, catalysis, and molecular inorganic photophysics. Within biology, RXES/RIXS has provided detailed insights into how cytochrome *c* can function as both an electron transfer protein in oxidative phosphorylation and a peroxidase enzyme in programmed cell death (i.e., apoptosis). In catalysis, RXES/RIXS is a powerful, site-selective probe of the electronic structures of heterogeneous catalysts and their molecular analogs and has provided insights into the mechanism of O–O bond formation in the electrocatalytic oxygen evolution reactivity of cobalt oxides. Lastly, we demonstrate the unique power of high-resolution L-edge RIXS to define the ligand field excited state manifolds of inorganic complexes, with an emphasis on the spin- forbidden, photochemically active electronic states of metal-metal quadruply-bonded Re_2 dimers. Generally, we further showcase the high-level insights that can be gained by coupling density functional theory and multiplet ligand field calculations to the unique information content of RXES and RIXS.

Wednesday, May 8

WK6 CNM:
Optoelectronic Devices and Mechanical Systems Based on Ultra-thin 2D Materials

Location: APCF Conference Room, Building 446

Time: 8:30 – 5:30

Organizers: Irma Kuljanishvili (St. Louis University) and Saptarshi Das (Penn State)

Workshop aims to facilitate and strengthen the synergetic approach to experimental and theoretical works of experts from academia, national labs and industries to discuss the latest developments in the synthesis, characterization, and application of ultra-thin 2D materials and device architectures with the emphasis to explore their unique potential as smart/adaptive devices, and substrate or other stimulus-responsive systems.

Properties of these layered 2D materials can be tuned by lateral confinements and vertical multi-layer z-stacking. This offers opportunity for development of next generation of multi-functional devices whose properties can be engineered/designed to specific performance. Particular emphasis would be on optoelectronic and mechanical systems.

The materials of interest include but not limited to van der Waals materials (graphene, hBN, and TMDC or other mono-elemental layered 2D systems and heterostructures). Recent advances in the development of 2D materials and understanding of their electronic, optical, mechanical or thermal, properties have demonstrated vast potentials in these systems.

Center for Nanoscale Materials at Argonne has expertise and state-of-the-art facilities in the synthesis, functionalization and characterization of 2D materials and has a strong research program focused around the fundamental studies on physical properties of these materials. Workshop will include topics covering fundamental physical aspects of 2D materials and heterostructures, their growth, characterization and applications. Computational modeling offers opportunity for computational experimentation and testing of physical, chemical and mechanical properties with emphases on manipulating interfaces of these layered materials by geometric al designs and/or surface interaction for targeted outcome and/or applications. The workshop will facilitate discussions that explore routes for scalable and transformative technologies.

This workshop is expected to provide an opportunity for academics, R&D scientists in industry, and students to exchange ideas, think creatively about new avenues for collaborations with user facilities at Argonne and to work on expanding knowledge of nanoscience into development and implementation of new frontiers in nanotechnology.

Workshop topics include:

- Advances in fabrication and characterization, of 2D materials and heterostructures with emphasis on fundamental science, and their potential for scalability and/or commercialization.
- Novel device architectures with emphasis on optoelectronic and mechanical systems made with 2D materials and heterostructures, their fundamental properties, manufacturing, and testing.
- Optoelectronic devices made with 2D heterostructures on flexible substrates, functional and adaptable optoelectronic and optomechanical devices.
- Computational studies interface designs, mechanical: Computational approach for understanding interfaces interactions and mechanical properties with emphases on interface engineering.

8:30 – 8:35	Opening Remarks
8:35 – 9:25	Jiwoong Park (University of Chicago) *Atomically Thin Materials for Technology*
9:25 – 10:15	Ali Javey (University of California at Berkeley) *Making Semiconductor Monolayers Perfectly Bright*
10:15 – 10:30	Break
10:30 – 11:20	Zhihong Chen (Purdue University) *2D Cu Diffusion Barriers for Ultra-scaled Interconnect Technologies*
11:20 – 12:10	Mark Hersam (Northwestern University) *Mixed-dimensional van der Waals Heterostructures for Electronic and Energy Applications*
12:10 – 1:40	Lunch
1:40 – 2:30	Philip Feng (Case Western Reserve University) *Atomic Layer Semiconductor and Heterostructure Nanoelectromechanical Systems for Information Processing*
2:30 – 3:20	Ani Sumant (Argonne National Laboratory) *Advances in Superlubricity Using Hybrid 2D Materials-based Lubricants*
3:20 – 3:40	Break
3:40 – 4:30	Xiaodong Xu (The University of Washington) *Moiré-excitons in $MoSe_2$/WSe_2 Heterobilayers*
4:30 – 5:20	Vikas Berry (University of Illinois-Chicago) *Chemical and Structural Manipulation of Graphene and Other 2D Nanomaterials for Electronics and Optoelectronics*
5:20 – 5:30	Closing Remarks
5:30	Adjourn

WK6

Atomically Thin Materials for Technology

Jiwoong Park

University of Chicago, Chicago, IL 60637

Manufacturing of paper, which started two thousand years ago, simplified all aspects of information technology: generation, processing, communication, delivery and storage. Similarly powerful changes have been seen in the past century through the development of integrated circuits based on silicon. In this talk, I will discuss how we can realize these integrated circuits thin and free-standing, just like paper, using two-dimensional inorganic and organic materials and how they can impact future technology. In order to build these atomically thin circuits, we developed a series of chemistry-based approaches that are scalable and precise. They include wafer-scale synthesis of three atom thick semiconductors and heterojunctions (*Nature*, 2015; *Science*, 2018), a wafer-scale patterning method for one-atom-thick lateral heterojunctions (*Nature*, 2012), and atomically thin films and devices that are vertically stacked to form more complicated circuitry (*Nature*, 2017). Once realized, these atomically thin circuits will be foldable and actuatable, which will further increase the device density and functionality.

WK6

Making Semiconductor Monolayers Perfectly Bright

Ali Javey

Electrical Engineering and Computer Sciences, University of California, Berkeley, CA 94720

Two-dimensional semiconductors exhibit excellent device characteristics, as well as novel optical, electrical, and optoelectronic characteristics. In this talk, I will present our recent advancements in surface passivation, contact engineering, surface charge transfer doping, and heterostructure devices of layered chalcogenides. We have developed a passivation technique that allows for observation of near-unity photoluminescence quantum yield in monolayer semiconductors. I will discuss the mechanism by which non-radiative recombination can be fully removed in monolayers. The work presents the first demonstration of an opto-electronically perfect monolayer, and highlights one of their unique properties. Finally, I will discuss an AC carrier injection mechanism to enable bright light emitting devices using monolayers, overcoming the problem of Schottky contacts.

WK6

2D Cu Diffusion Barriers for Ultra-scaled Interconnect Technologies

Zhihong Chen

School of Electrical and Computer Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907

Cu is used as the interconnect material in IC chips because of its superior conductivity. However, the diffusion of Cu into the dielectric between two interconnects can cause shorting and create chip failures, while the diffusion to transistors can introduce deep-level traps to Si and affect the transistor performance. Ta/TaN bilayer stacks have been used as diffusion barrier/liner materials to isolate Cu from surrounding intra/inter-layer dielectrics. Along with the scaling of VLSI, the dimensions of interconnects and vias need to be scaled as well. To maximize Cu volume for lower line resistance and reduce thevia resistance, the thickness of the barrier/liner bilayer should be scaled accordingly. However, these materials lose their capability of blocking Cu diffusion as their thickness is extremely reduced. In this talk, I will show that the diffusion barrier and liner properties of several 2D materials are investigated by various characterization methods. We observe that the lifetime of the dielectrics surrounding Cu electrodes can be significantly extended with the presence of the tested 2D barriers, providing strong evidence for promising alternative barrier/liner solutions.

WK6

Mixed-dimensional van der Waals Heterostructures for Electronic and Energy Applications

Mark C. Hersam

Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208

Layered two-dimensional (2D) nanomaterials interact primarily via van der Waals bonding, which has created new opportunities for heterostructures that are not constrained by epitaxial growth [1]. However, it is important to acknowledge that van der Waals interactions are not limited to interplanar interactions in 2D materials. In principle, any passivated, dangling bond-free surface interacts with another via non-covalent forces. Consequently, the emerging layered 2D nanomaterials can be integrated with a diverse range of other materials, including those of different dimensionality, to form mixed-dimensional van der Waals heterostructures [2]. In order to efficiently explore the vast phase space for mixed-dimensional heterostructures, our laboratory employs solution-based additive assembly [3]. In particular, constituent nanomaterials (e.g., carbon nanotubes, graphene, transition metal dichalcogenides, black phosphorus, boron nitride, and indium selenide) are isolated in solution, and then deposited into thin films with scalable additive manufacturing methods (e.g., inkjet, gravure, and screen printing) [4]. By achieving high levels of nanomaterial monodispersity and printing fidelity [5], a variety of electronic and energy applications can be enhanced including digital logic circuits [6], photodetectors [7], and lithium-ion batteries [8]. Furthermore, by integrating multiple nanomaterial inks into heterostructures, unprecedented device function is realized including anti-ambipolar transistors [9], gate-tunable photovoltaics [10], and neuromorphic memtransistors [11]. In addition to technological implications for electronic and energy technologies, this talk will explore several fundamental issues including band alignment, doping, trap states, and charge/energy transfer across previously unexplored mixed-dimensional heterointerfaces [12].

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WK6

Atomic Layer Semiconductor and Heterostructure Nanoelectromechanical Systems for Information Processing

Philip Feng

Electrical Engineering, Case School of Engineering, Case Western Reserve University, Cleveland, OH 44106

Atomically thin crystals (including semiconducting, metallic and insulating layers) and their heterostructures offer compelling new platforms for 2D electronic, photonic devices and nanoelectromechanical systems (NEMS), where their unconventional and unique properties can be harnessed for engineering both classical signal processing and quantum transduction schemes. In this presentation, I will describe some of my research group's latest effort on advancing device physics and engineering of 2D heterostructures and NEMS. I will first show atomically thin radio-frequency (RF) NEMS resonators with excellent electrical tunability and remarkably broad dynamic range. I will then demonstrate how the unusually strong and efficient coupling effects have led to ultra-broad resonance tuning of van der Waals heterostructure resonators, as well as stable, robust graphene NEMS operating at glowing temperatures with simultaneous light emission. I will also describe h-BN nanomechanical resonators and phononic waveguides, as well as other 2D building blocks, and device engineering effort on new, energy-efficient signal transduction and information processing, toward realizing chip-scale integrated platforms.

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WK6

Advances in Superlubricity Using Hybrid 2D Materials-based Lubricants

Anirudha V. Sumant

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Recent advances in achieving near zero friction at macroscale in sliding interfaces using solid lubricants based on 2D materials-nanoparticles hybrid combination opened new possibilities for reducing wear and friction related losses in various mechanical systems involving rotational/sliding motion [1]. The energy loss due to wear and friction in moving mechanical systems amounts to quarter of total energy loss worldwide. Oil-based lubricants used in majority of moving mechanical system have to be either spent (burned) or dumped into the environment after their use, creating major problems to the environment. Various alternatives including bio-degradable oil are being developed; however, more effort and research is needed to develop green lubricants.

Our recent work on utilizing combination of 2D materials (such as graphene and MoS_2) with nanodiamond as an oil-free lubricant have shown that we can achieve superlubricity (near zero friction) as well as exceptional wear resistance of the sliding components, at macroscale [2,3]. This discovery presents a paradigm shift from conventional oil-based lubrication and allows us to explore untapped potential of nanomaterials as a dry solid lubricant in many rotational/sliding mechanical systems. We show that near zero friction is possible due to structural reorganization in case of graphene-nanodiamond forming nanoscale ball-bearings and formation of onion-like-carbon (OLC) in case of MoS_2 and nanodiamond through tribochemical reaction at the sliding interface. The formation of OLCs is self-generating providing unlimited supply of lubricant and thus helping to increase the wear-life significantly.

I'll discuss the detailed experimental studies along with theorical investigations that suggest the overall mechanism of superlubricity. I'll also discuss our efforts towards commercializing this technology by working collaboratively with industry.

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WK6

Moiré-excitons in $MoSe_2/WSe_2$ Heterobilayers

Xiaodong Xu

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The creation of moiré patterns in crystalline solids is a powerful approach to manipulate their electronic properties, which are fundamentally influenced by periodic potential landscapes. In two-dimensional (2D) materials, a moiré pattern with a superlattice potential can form by vertically stacking two layered materials with a twist and/or finite lattice constant difference. This unique approach has led to emergent electronic phenomena, including the fractal quantum Hall effect [1–3], tunable Mott insulators [4,5], and unconventional superconductivity [6]. Furthermore, theory predicts intriguing effects on optical excitations by a moiré potential in 2D valley semiconductors [7–9], but these signatures have yet to be experimentally detected. In this talk, I will report our experimental evidence of interlayer valley excitons trapped in a moiré potential in $MoSe_2/WSe_2$ heterobilayers. We observe quantum-dot-like photoluminescence of interlayer excitons with the inheritance of unique valley-contrasting properties from the heterobilayer bulk. Twist angle dependent studies further support our observation of moiré excitons. Our results open opportunities for 2D moiré optics with twist angle as a unique control knob.

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WK6

Chemical and Structural Manipulation of Graphene and Other 2D Nanomaterials for Electronics and Optoelectronics

Vikas Berry

Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL 60607

The presentation will outline several chemical and structural manipulation techniques developed in our laboratory to control the properties of 2D nanomaterials. (a) Structural manipulation includes formation of wrinkles, nanoribbons and quantum dots, and (b) Chemical manipulation includes non-destructive functionalization, nanoparticle incorporation and biomolecular interfacing. The following topics will be discussed: (i) selective desiccation of bacterium under impermeable and flexible graphene *via* a flap-valve operation to produce axially-aligned graphene-wrinkles with anisotropic electrical properties; (ii) nanotomy process to cleave graphite nanoblocks and their exfoliation to produce graphene nanostructures (nanoribbons and quantum dots) with controlled electrical properties; (iii) wrinkling of MoS_2 to control photoluminescence; (iv) unique eta-6 organometallic approach to functionalize graphene in a vapor-phase process, while retaining its structural and electrical properties and offering chemical sites for nano-interfacing of plasmonic centers for enhanced photovoltaics; (v) biointerfacing of graphene and MoS_2 with cancer cells and bacteria for bionanotechnology and biomedical applications; and (vi) Photovoltaics via electronic coupling of graphene atop a bulk semiconductor to induce interfacial energy-band reorganization for light-sensitive junctions only one atom below the front surface.

Tuesday, May 7

WK7 APS: *In Situ* and Multimodal Microscopy for APS-U

Location: Building 446, Conference Room

Time: 8:30 – 5:00

Organizers: Ross Harder (APS XSD), Jörg Maser (APS XSD), Wonsuk Cha (APS XSD), and Michael Stuckelberger (DESY)

The Upgrade of the Advanced Photon Source with a multi-bend achromat magnetic lattice will revolutionize coherent imaging and microscopy techniques with significantly improved spatio-temporal resolution, greater sensitivity to a variety of contrast mechanisms, and multimodal imaging capabilities.

With x-ray fluorescence beginning to be sensitive to just a handful of atoms in an illuminated volume and coherent imaging reaching down to length scales approaching single atomic crystallographic defects, there is tremendous opportunity for cross-platform and in situ studies of materials across many decades of length scales in the suite of planned instruments at the APS. Examples are the study of individual catalytically active particles, study of photovoltaic and battery materials and devices, and study of evolution and kinetics during materials synthesis, operation, and degradation.

Accomplishing truly cross-platform investigations of individual samples will require the development of *in situ* instruments and methodology compatible with the many imaging, microscopy and spectroscopy instruments planned for the APS Upgrade. This workshop will bring together both domain experts and instrument scientists working at the forefront of *in situ* and *operando* x-ray characterization to identify high-impact opportunities for cross-platform and multimodal investigations.

8:30 – 8:45 Introduction

8:45 – 9:30 Michael Stuckelberger (Deutsches Elektronen Synchrotron DESY)
In Situ *Meets* Operando *Meets Multi-modal: Opportunities and Challenges of X-ray Microscopy for Solar Cells*

9:30 – 10:15 Andrej Singer (Cornell University)
Nucleation of Dislocations and Their Dynamics in Layered Oxides Cathode Materials during Battery Charging

10:15 – 10:45 Break

10:45 – 11:30 Amelie Rochet (Brazilian Synchrotron Light Laboratory, LNLS)
Coherent X-ray Diffraction Imaging Unravelling Structure-activity Relationships of Gold Catalysts

11:30 – 12:30 Sebastian Kalbfleisch (MAX IV Laboratory, Lund University)
The NanoMAX Beamline at MAX IV

12:30 – 1:30 Lunch

1:30 – 2:15	Paul Evans (University of Wisconsin, Madison) *Expanding the Scope of Nanobeam Diffraction: Dynamical Diffraction in Epitaxial Electronic Materials*
2:15 – 2:35	Junjing Deng (Argonne National Laboratory) *Correlative X-ray Ptychographic and Fluorescence Imaging at the Advanced Photon Source*
2:35 – 3:00	Christian Roehrig (Argonne National Laboratory) In Situ *and Multimodal Microscopy for APS-U Workshop*
3:00 – 3:30	Break
3:30 – 4:15	Richard Sandberg (Los Alamos National Laboratory) *Studying Materials Deformation and Failure with Bragg Coherent Diffraction Imaging*
4:15	Changyong Park (Argonne National Laboratory) *Challenges in* In Situ *Observation of Texture and Microstructure Evolution of Polycrystals under Pressure with Diffraction-based Imaging and Microscopy Techniques*

WK7

In Situ Meets *Operando* Meets Multi-modal: Opportunities and Challenges of X-ray Microscopy for Solar Cells

Michael E. Stuckelberger[1,2], Christina Ossig[1,3], T. Nietzold[2], Mariana. I. Bertoni[2], and Christian G. Schroer[1,3]

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Today, we are utilizing scanning probe x-ray microscopy endstations at 3rd generation synchrotrons to answer questions about photovoltaic materials such as: How do interfaces look like in solar cell stacks? How can thin-film devices be manufactured without sacrificing the efficiency due to lateral inhomogeneity? Which defects limit the device performance, and how can they be engineered to be less detrimental? How can solar cells be cost-effectively fabricated using abundant and non-toxic materials?

Based on experiments at DESY, APS, ESRF, and NSLS II, we will showcase examples of multimodal solar cell measurements during *in situ* growth and operation of solar cells, involving x-ray beam induced current (XBIC) and voltage (XBIV), x-ray fluorescence (XRF), x-ray diffraction (XRD), ptychography, and x-ray excited optical luminescence (XEOL). We have found correlations between the optical / electrical performance, composition, and strain, and will highlight the significance of correlations between performance and material properties for the solar cell development.

Tomorrow, the questions will be different, and we will be able to use x-ray microscopes at 4th generation synchrotrons to answer them. Where the frontiers of scanning microscopy will be pushed to? Which challenges arise with the new opportunities, and how can we tackle them? We will present ideas of 'dream experiments' and discuss the challenges related to multimodal scanning x-ray microscopy.

WK7

Nucleation of Dislocations and Their Dynamics in Layered Oxides Cathode Materials during Battery Charging

Andrej Singer

Department of Materials Science and Engineering, Cornell University, Ithaca, NY 14853

Lithium-rich layered oxides (LRLO) are among the leading candidates for the next generation cathode material for energy storage, delivering 50% excess capacity over commercially used compounds. Despite excellent prospects, voltage fade has prevented effective use of the excess capacity, and a major challenge has been the lack of understanding of the mechanisms underpinning the voltage fade. I will present our recent results, where using *operando* three-dimensional Bragg coherent diffractive imaging, we directly observe the nucleation of a mobile dislocation network in LRLO nanoparticles. The dislocations form more readily in LRLO as compared with a classical layered oxide, suggesting a link between the defects and voltage fade. We show microscopically how the formation of partial dislocations contributes to the voltage fade. The insights allow us to design and demonstrate an effective method to recover the original high voltage functionality.

Our findings reveal that the voltage fade in LRLO is reversible and call for new paradigms for improved design of oxygen-redox active materials.

WK7

Coherent X-ray Diffraction Imaging Unravelling Structure-activity Relationships of Gold Catalysts

Amélie Rochet

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Chemical properties of catalytic materials are dependent on dynamic changes of the three-dimensional structure of the catalysts as well as the reactive environment. The active sites formed under reaction conditions are short-lived species and their identification remains a great challenge. Besides, defects and lattice strain dynamics of nanocrystals directly tuned their catalytic properties. To understand the nature of the active sites and the relationship between catalysts structure and activity, the study of catalysts under *operando* conditions is crucial. Bragg coherent x-ray diffraction imaging (BCDI) provides a unique opportunity to follow in 3D under realistic reaction conditions the strain and defects dynamics in the surface and inner core of the nanomaterials.

In this talk, I will present our *in situ/operando* BCDI investigations of gold catalysts during CO oxidation. Under the catalytic reaction conditions, we investigate the defects dynamics of gold nanocrystals with twin domains and show the *in situ* formation of a nanotwin network that correlates with the catalytic properties. Besides, we follow at the single nanoparticle-level, the highly dynamic 3D strain distribution during the hysteresis phenomenon occurring through CO oxidation reaction cycles.

WK7

The NanoMAX Beamline at MAX IV

Sebastian Kalbfleisch, Ulf Johansson, Gerardina Carbone, and Alexander Björling

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The MAX IV synchrotron has started operation during 2016 and its 3 GeV ring is considered pioneering in the world of diffraction limited sources. One of the beamlines which stands to profit most is the NanoMAX beamline [1], a hard x-ray nanoprobe, set for best performance between 8 and 15 keV. It exploits especially the low vertical emittance of the ring by employing a horizontal Bragg diffracting crystal Si(111) monochromator, used to select the working energy in the range 6–20 keV, and a 1:1 focusing scheme of the source size on the secondary source aperture (SSA) placed at 51m from the undulator, allowing full control of flux versus coherence. A superpolished KB-mirror pair is used to focus the light onto the sample at 98m, with an energy dependent spot size: from 200 nm at 5 keV, down to 50 nm at 20 keV. With SSA settings optimized for coherence, the beamline delivers a maximum flux of around 1E10 on the sample.

In this talk, we will highlight some of the characteristics of the beamline, as well as present results from various types of experiments (e.g., forward ptychography and CDI, scanning diffraction and coherent imaging in Bragg geometry, x-ray fluorescence) performed at the first of two planned end-stations taken during the beamline's first two years of operation.

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WK7

Expanding the Scope of Nanobeam Diffraction: Dynamical Diffraction in Epitaxial Electronic Materials

Paul G. Evans

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Epitaxial electronic materials include a thin film or nanostructure that shares key aspects of its crystallographic structure with a thick underlying substrate. In key applications of these epitaxial materials in the development of semiconductor quantum computing, the control of this structure at the scale of tens to hundreds of nanometers has been an important challenge. Semiconductor quantum computing devices based on heterostructures formed in the AlGaAs/GaAs system involve thin epitaxial layers with tiny lattice mismatches on the order of 10^{-4} or smaller and rely on the formation of qubits defined at the lateral scale of tens of nanometers. The further mechanical distortion of these layers during the formation of devices causes significant electronic perturbations due to the piezoelectric and deformation potential effects. Ultimately, the mechanical distortion and the accompanying electronic perturbation affects the operation of devices. It has been challenging, however, to characterize the mechanical distortion of these epitaxial layers, in part because the close lattice match between the substrate and the thin film has posed a difficult problem for x-ray nanobeam diffraction techniques. We have found that this problem can be addressed through the development of new nanobeam diffraction methods in which dynamical diffraction simulations are employed to interpret the complex diffraction patterns arising from latticed-matched heterostructures [1].

Nanobeam diffraction studies of lattice-matched GaAs/AlGaAs quantum computing devices reveal mechanical

distortions due to device fabrication, including from the residual stress and thermal expansion coefficient mismatch associated with metallic electrodes [2,3]. This new understanding the magnitude and role of these effects has the potential to allow the design of improved device geometries and potentially to lead to devices in which strain, in addition to electrostatic effects, is used to define quantum devices.

Beyond quantum computing structures, similar dynamical diffraction effects appear in problems associated with ferroelectric domains and domain boundaries in epitaxial $BaTiO_3$ thin films and in strain sharing effects in nanoscale complex oxides [4].

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WK7
Correlative X-ray Ptychographic and Fluorescence Imaging at the Advanced Photon Source

Junjing Deng[1], Si Chen[1], Yudong Yao[1], Yi Jiang[1], Qiaoling Jin[2], Chris Jacobsen[1,2,3], Zhonghou Cai[1], Barry Lai[1], and Stefan Vogt[1]

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Accurate knowledge of elemental distributions of specimens within their structural context is very important for understanding their roles and the resulting sample behaviors. At the Advanced Photon Source (APS), we have developed a correlative imaging method via a combination of x-ray fluorescence microscopy (XFM) and ptychography [1,2]. XFM offers high sensitivity for quantitative mapping of elements in samples with a spatial resolution that limited by beam size, while ptychography provides a complementary approach to visualize ultrastructure beyond focusing-optic resolution limit. We have applied this correlative method on the study of materials samples including solar cell film [3] and electrocatalysts [4], as well as 3D frozen-hydrated cells [5]. To speed up the imaging speed, we have developed photon-efficient fly-scan techniques [6] together with novel instrumentations [7]. By using continuous scanning, novel data analysis, and a new generation of synchrotron light source provided by APS-U, it will enable high-throughput high-resolution imaging which provides opportunities to implement this correlative tool for *in situ* and *operando* measurements.

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.

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WK7
In Situ and Multimodal Microscopy for APS-U Workshop

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The increased coherent flux that will become available with the APS Upgrade will provide exciting opportunities for new types of experiments. Critical to the realization of these experiments are instruments that are able to handle a variety of scan trajectories, have sufficient precision and bandwidth, and provide for the high-speed collection of both position and x-ray data. These goals necessitate control systems that are flexible and dynamic and built upon robust mechanics and position metrology. In this talk, I will discuss the current development efforts at the APS on scanning microscopes. I will then talk about performance targets for some of the APS Upgrade beamline control systems and the challenges that must be met to get there.

WK7

Studying Materials Deformation and Failure with Bragg Coherent Diffraction Imaging

Richard L. Sandberg[1], Mathew J. Cherukara[2], Reeju Pokharel[3], Timothy O'Leary[1], Jonathan Gigax[1], Eric E. Hahn[3], Wonsuk Cha[2], Ross J. Harder[2], and Saryu J. Fensin[3]

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We are developing Bragg coherent diffraction imaging (BCDI) to study materials damage and failure in structural metals. BCDI can provide nanometer scale images of strain in crystalline materials. Our team performed the first proof of principle demonstration of combined *in situ* BCDI experiment guided by MD diffraction simulations on a thin film specimen of deformed copper [1]. We are developing compatible tensile and compressive loading cells to stress materials at the nanometer scale. We are also developing a tuneable monochromator for the coherent x-ray scattering beamline at APS (34ID-C) as part of a partner user proposal to conduct in-situ orientation mapping of polycrystalline thin films, thus enabling more rapid identification of desired nanocrystals or grains. Finally, we are also studying materials implanted with helium ions as a way to understand how materials in nuclear reactors lose strength under high radiation environments. Techniques such as these may enable us to understand materials damage in reactors.

This work was supported by the U.S. Department of Energy (DOE) at Los Alamos National Laboratory (LANL) under Contract No. DE-AC52-06NA25396 through the LANL LDRD Program 20180683ER and the Institute for Materials Science 2016 Rapid Response program. We also acknowledge funding support from the LANL Dynamic Materials Campaign (C2). This work was also supported by Argonne National Laboratory LDRD 2015-149-R1 (Integrated Imaging, Modeling, and Analysis of Ultrafast Energy Transport in Nanomaterials) and Argonne National Laboratory LDRD 2018-019-N0 (A.I. C.D.I: Atomistically Informed Coherent Diffraction Imaging).

The experiment was performed at the 34-IDC beamline of the Advanced Photon Source (APS). This work was supported, in part, by the Center for Nanoscale Materials. The Advanced Photon Source, the Center for Nanoscale Materials and the Argonne Leadership Computing Facility are supported by the U.S Department of Energy, Office of Science, Office of Basic Energy Sciences (BES), under Contract No. DE-AC02-06CH11357. The work was in part supported by the Center for Integrated Nanotechnologies, a U.S. DOE BES user facility.

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WK7

Challenges in *In Situ* Observation of Texture and Microstructure Evolution of Polycrystals under Pressure with Diffraction-based Imaging and Microscopy Techniques

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Textures and microstructures of polycrystals evolve with compression, resulting in nonuniformity in the strain distributions and phase equilibria. While the anisotropy is readily expected under non-hydrostatic conditions, recent observations of the high-pressure micro-XRD using diamond anvil cells show more and more evidences for inherently anisotropic responses of polycrystals to the external pressure even under hydrostatic conditions. The nonuniformity of strain distribution under hydrostatic compression raises a fundamental question to determining isothermal equation of state of crystalline solids and to describing the macroscopic behaviors as to be thermodynamically equilibrated phases.

The intergranular interactions that are responsible to dynamically changing textures with external pressure seem to be intimately correlated with the intragranular response to the local forces forming anisotropic strain fields inside single grains. Shear-induced phase transition can be triggered by this localized deformation processes, which in turn further complicates the microstructure evolution. The microscopic (nucleation and growth) to mesoscopic (intragranular development) to macroscopic (texture and microstructure evolution and phase equilibria) link is extremely difficult to observe *in situ* due to the orders of magnitude changes in its scale but has yet to be fully described to better model the predictable phase behaviors under compression.

The spatially resolved x-ray diffraction imaging and microscopy would be required to address these highly localized phenomena. Some x-ray diffraction-based imaging techniques are promising for *in situ* observations of the pressure-induced local variations, but there are several challenges to be overcome for the successful applications. In this presentation, a case of pure Zr polycrystal is presented with the results of 2D x-ray diffraction imaging (XDI) and grain Bragg coherent diffraction imaging (gBCDI). The challenges involved in the technical development and the future perspectives are discussed.

Portions of this work were performed at HPCAT (Sector 16), 1-ID-E, and 34-ID-C beamlines, Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences. The Advanced Photon Source is 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.

POSTER INDEX

Posters are indexed according to first author last name

Advanced Photon Source

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, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

Biology

A1	Anton Frommelt	LRL-CAT: An Automated X-ray Crystallography Synchrotron Beamline for Structure-based Drug Design
A2	D.J. Kissick	Improvements in Serial Crystallography Capabilities at GM/CA
A3	Anna Shiriaeva	Ligand Exchange Method for High-throughput Crystallization of Novel Ligand-GPCR Complexes
A4	Michael Vega	Investigating the Effect of Cholesterol on Supported Lipid Bilayers of Dipalmitoylphosphatidylcholine

Chemistry

A5	Roman Ezhov	New Pathways in Iron-based Water Oxidation Catalysis
A6	Jicheng Guo	High Energy SAXS-WAXS Studies on the Fluid Structure of Molten LiCl-Li Solutions
A7	Scott C. Jensen	Understanding X-ray Spectroscopic Signatures of Photosystem II Using Mn Coordination Complexes
A8	Anthony Krzysko	Breakage and Restructuring of Boehmite Aggregates Analyzed by *in situ* Capillary Rheometry, Ultra-small Angle, Small Angle, and Wide Angle X-ray Scattering
A9	Zhu Liang	Tracing Ion Concentrations in Back-extraction Processes via X-ray Fluorescence near Total Reflection
A10	Kaitlin Lovering	Surface Sensitive Spectroscopy for Understanding Liquid-liquid Extraction
A11	Lu Ma	X-ray Absorption Spectroscopy for Single-atom Catalysts at 9-BM
A12	Anne Marie March	Synchrotron Hard X-ray Spectroscopic Investigation of the Photoaquation Reaction Mechanism in Hexacyanoferrate(II) with Sub-pulse Temporal Resolution
A13	Debora Meira	*In situ* Experiments Using Synchrotron Techniques

A14	Srikanth Nayak	Structural Analysis in Soft Matter Using Synchrotron X-ray Scattering Techniques
A15	Marek Piechowicz	Amidoxime-functionalized Ultra-high Porosity Materials for ^{230}Th and ^{233}U Separations
A16	Ming-Feng Tu	Micro-focused MHz Pink Beam for Time-resolved X-ray Emission Spectroscopy
A17	Qi Wang	Probing Open Metal Sites in High Valence Metal-organic Frameworks by *in situ* Single Crystal X-ray Diffraction
A18	Tianpin Wu	Investigations of Catalysis and Batteries at Beamline 9-BM: Capabilities and Upgrade

Environmental Science and Geology

A19	Hassnain Asgar	Understanding the Morphological Evolution in CO_2-responsive Nanofluids during the Hydrogel Formation Using Time-resolved USAXS/SAXS Measurements
A20	Clara R. Ervin	Identifying Poultry Litter Ash Phosphorus Speciation and Submicron Structure Composition Effect on Efficiency as a Maize Fertilizer
A21	Seungyeol Lee	The Role of Nano-interface of Hemoilmenite in Enhancing Remanent Magnetization
A22	Dien Li	Iodine Immobilization by Silver-impregnated Granular Activated Carbon in Cementitious Systems
A23	Lauren Mosesso	Understanding P Dynamics of Delmarva Peninsula “Legacy” P Soils by X-ray Absorption Near Edge Structure Spectroscopy (XANES)

High Pressure

A24	Stella Chariton	Single-crystal X-ray Diffraction at Extreme Conditions

Instrumentation

A25	Anasuya Adibhatla	Recent Developments in BIO-SAXS Using MetalJet X-ray Source
A26	Tolulope M. Ajayi	Commissioning of XTIP Beamline at the Advanced Photon Source
A27	Sergey P. Antipov	Status of the Diamond CRL Development

A28	Sergey V. Baryshev	Mega-electron Volt *Lab-in-Gap* Time-resolved Microscope to Complement APS-U: Looking into Solid State Chemistry for Energy Applications
A29	Pice Chen	Ultrafast Hard X-ray Modulators Based on Photonic Micro-systems
A30	Steve Heald	Advanced Spectroscopy and LERIX Beamlines at Sector 25 for APSU
A31	Steven P. Kearney	A Comparison of Isolated and Monolithic Foundation Compliance and Angular Vibrations
A32	Samuel D. Marks	Combined Scanning Near-field Optical and X-ray Diffraction Microscopy: A New Probe for Nanoscale Structure-property Characterization
A33	U. Patel	Development of Transition-edge Sensor X-ray Microcalorimeter Linear Array for Compton Profile Measurements and Energy Dispersive Diffraction
A34	Curt Preissner	(The) RAVEN at 2-ID-D
A35	Carl Richardson	Direct LN2-cooled Double Crystal Monochromator
A36	M.L. Rivers	areaDetector: What's New?
A37	Valeri D. Saveliev	Vortex-ME7 SDD Spectrometer: Design and Performance
A38	Andreas Schacht	Sub-20-nrad Stability of LN_2-cooled Horizontal and Vertical Offset Double-crystal Monochromators
A39	D. Shu	Mechanical Design and Test of a Capacitive Sensor Array for 300-mm Long Elliptically Bent Hard X-ray Mirror with Laminar Flexure Bending Mechanism
A40	Chengjun Sun	Machine Learning Enabled Advanced X-ray Spectroscopy in the APS-U Era
A41	Shaoze Wang	UHV Optical Chopper and Synchrotron X-ray Scanning Tunneling Microscopy Implementation

Materials Science

A42	Shengyuan Bai	X-ray Topography and Crystal Quality Analysis on Single Crystal Diamond Grown by Microwave Plasma Assisted Chemical Vapor Deposition
A43	Arun J. Bhattacharjee	*In situ* X-ray Tomography of Pack Cementation for Analysis of Kirkendall Porosity Formed during Titanium Deposition on Nickel Wires
A44	Wonsuk Cha	*In situ* and *Operando* Bragg Coherent Diffractive Imaging at APS 34-ID-C

A45	Amlan Das	Stress-driven Structural Dynamics in a Zr-based Metallic Glass
A46	V. De Andrade	Fast *in situ* 3D Characterization of Nano-materials with X-ray Full-field Nano-tomography: Latest Developments at the Advanced Photon Source
A47	Ramón D. Díaz	Measuring Relative Crystallographic Misorientations in Mosaic Diamond Plates Based on White Beam X-ray Diffraction Laue Patterns
A48	Ankit Kanthe	Understanding the Dynamics of Mabs and Excipients at the Air-water Interface
A49	Kamil Kucuk	Carbon-coated High Capacity Li-rich Layered $Li[Li_{0.2}Ni_{0.2}Mn_{0.5}Fe_{0.1}]O_2$ Cathode for LIBs
A50	Saman Moniri	The Mechanism of Eutectic Modification by Trace Impurities
A51	Jesse Murillo	Single Molecule Magnetic Behavior of Near Liner N,N Bidentate Dy Complex
A52	Andrei Tkachuk	Non-destructive 3D Grain Mapping by Laboratory X-ray Diffraction Contrast Tomography
A53	Hua Zhou	Investigating Atomic Structures of Mesoscale and Highly Curved Two-dimensional Crystals by Surface X-ray Nanodiffraction

Nanoscience and Nanotechnology

A54	Alexandra Brumberg	Photoinduced, Transient Disordering in CdSe Nanostructures Characterized via Time-resolved X-ray Diffraction (TR-XRD)
A55	Yuxin He	GI-S/WAXS Study of the Effects of Silica Nanopore Confinement and Tethering on Crystallization and Transport Behavior of 1-butyl-3-methylimidazolium [BMIM]-based Ionic Liquids
A56	Prabhat KC	Convolutional Neural Network Based Super Resolution for X-ray Imaging

Technique

A57	Mrinal Bera	A Dedicated ASAXS Facility at NSF's ChemMatCARS
A58	Wei Bu	Liquid Surface/Interface Scattering Program at NSF's ChemMatCARS
A59	Eran Greenberg	Python Software Development at GSECARS
A60	Saugat Kandel	On the Use of Automatic Differentiation for Phase Retrieval

A61	A.T. Macrander	Strain Mapping in Single Crystals from Maps of Rocking Curves at Beamline 1-BM of the Advanced Photon Source
A62	Lynn Ribaud	Synchrotron Powder Diffraction Simplified: The High-resolution Diffractometer 11-BM at the Advanced Photon Source

Center for Nanoscale Materials

Use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Chemistry

C1	Ravindra B. Weerasooriya	Photoregeneration of Biomimetic Nicotinamide Adenine Dinucleotide Analogues via a Dye-sensitized Approach

Condensed Matter Physics

C2	Dali Sun	Spintronic Terahertz Emission by Ultrafast Spin-charge Current Conversion in Organic-inorganic Hybrid Perovskites/Ferromagnet Heterostructures

Instrumentation

C3	Tejas Guruswamy	Hard X-ray Transition Edge Sensors at the Advanced Photon Source
C4	Daikang Yan	A Two-dimensional Resistor Network Model for Transition-edge Sensors with Normal Metal Features
C5	Jianjie Zhang	Superconducting Thin Films for Ultra-low Temperature Transition Edge Sensors

Materials Science

C6	Aida Amroussia	Ion Irradiation Damage in Commercially Pure Titanium and Ti-6Al-4V: Characterization of the Microstructure and Mechanical Properties
C7	Sahithi Ananthaneni	Electrochemical Reduction of CO_2 on Transition Metal/P-block Compositions
C8	Frank Barrows	Fabrication, *in situ* Biasing, Electron Holography and Elemental Analysis of Patterned and Unpatterned TiO_2 Thin Films
C9	Mason Hayward	Characterization of Boron/Iron-oxide Core/Shell Structure for Boron Neutron Capture Therapy by STEM/EELS-XEDS and Mössbauer Spectroscopy

C10	Megan O. Hill	Total Tomography of III-As Nanowire Emitters: Correlating Composition, Strain, Polytypes, and Properties
C11	Yu Jin	Structural Changes of Layered Optical Nanocomposites as a Function of Pulsed Laser Deposition Conditions
C12	Boao Song	*Operando* TEM Investigation of Sintering Kinetics of Nanocatalysts on MoS_2 in Hydrogen Environment
C13	Zhizhi Zhang	Manipulation of Spin Wave Propagation in a Magnetic Microstripe via Mode Interference

Nanoscience and Nanotechnology

C14	Zhaowei Chen	Light-gated Synthetic Protocells for Plasmon-enhanced Solar Energy Conversion
C15	Israel Hernandez	On the Homogeneity of TiN Kinetic Inductance Detectors Produced through Atomic Layer Deposition
C16	Devon Karbach	Mask Free Patterning of Custom Inks for Controlled CVD Growth of Two-dimensional Crystalline MoS_2 and WS_2 Semiconductors
C17	Yiming Li	Folding, Self-assembly and Characterization of Giant Metallo-supramolecules with Atomic Resolution
C18	Jonathan M. Logan	Optimizing the Design of Tapered X-ray Fesnel Zone Plates Using Multislice Simulations
C19	Hisham A. Maddah	Random Sampling of Ionic Radii and Discrete Distributions for Structural Stability and Formability of Titanium-based Perovskites
C20	Olga V. Makarova	Fabrication of High-aspect-ratio Gold-in-silicon X-ray Gratings
C21	Nicolaie Moldovan	Fluid-based Capillary Compound Refractive Lenses for X-ray Free Electron Lasers
C22	Nicholas Schaper	Engineering Nano-biocomposite Materials Using CNTs and ZnO Hybrid Interfaces and Hydrogel Environments for Future Biomedical Applications
C23	Prabhjot Singh	Characterization of 3D Printed Lab on Chip Structures for Cell Culture Applications
C24	Anuj Singhal	Applications of Sequential Infiltration Synthesis (SIS) to Structural and Optical Modifications of 2-photon Stereolithographically Defined Microstructures

C25	Michael Vogel	Temperature Dependent Skyrmion Hall Angle in Ferrimagnets
C26	Jiaxi Xiang	Selectivity through Morphology: Towards Highly Sensitive MOX/CNT Based Hydrocarbon VOC Sensors
C27	Xin Xu	Direct Grain Boundary Study in Cerium Oxide

Exemplary Student Research Program

Using the world-class facilities at Argonne's Advanced Photon Source, area high school students and their teachers explore the principles and operation of these tools and conduct research during the school year. Under the guidance of staff scientists, each team develops an achievable project based on the techniques and limitations within a specific research group, prepares and submits a research proposal, sets up the experiment, gathers and analyzes their results, draws conclusions, and prepares a final poster for the Users Meeting.

ESRP1	Bolingbrook High School	Local Structural Studies of Pd Based Catalytic Nanoparticles
ESRP2	Glenbard East High School	The Characterization of Phytochelatins Mediating Zinc Transport in *Arabidopsis thaliana*
ESRP3	Glenbrook South High School	Local Structure Analysis of Chromophore $YGa_{1-x}Mn_xO_3$
ESRP4	Hoffman Estates High School	Examining the Crystallization of Gold Nanoparticles Based on Variable Surface Pressure
ESRP5	Lemont High School	Root Uptake of Chromium and Nickel in Common Plants and Vegetables
ESRP6	Lincoln-Way East High School	Study of Ferrous Sulfate Oxidation under Extreme Conditions Using X-ray Absorption Spectroscopy
ESRP7	Lockport Township High School	Optimizing Data Collection at Beamline 17-ID Using Bovine Insulin
ESRP8	Naperville Central High School	Copper Oxidation States Found in Wood Preservatives and Their Relationship to Corrosion Factors
ESRP9	Neuqua Valley High School	Study of Industrial Metals in Soils Collected from Chicago Residential Areas
ESRP10	Romeoville High School	Testing Graphene as a Protective Coating for $LiMnO_2$ Batteries

APS POSTER ABSTRACTS

Biology

A-1

LRL-CAT: An Automated X-ray Crystallography Synchrotron Beamline for Structure-based Drug Design

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Eli Lilly and Company, Lemont, IL 60439

Eli Lilly and Company operates its own fully automated x-ray macromolecular crystallography beamline, LRL-CAT, on sector 31 of the Advanced Photon Source (APS) of Argonne National Laboratory. LRL-CAT runs exclusively as a mail-in facility for protein crystallography, providing crystallographic diffraction data for Lilly, its corporate partners, and general users of the APS. An expert, full-time staff maintains the beamline, monitoring the automated diffraction measurements and intervening manually when needed to provide the best data from each group of crystals. Users receive the data as soon they are collected and processed.

Eli Lilly is committed to maintaining and improving the high throughput, high quality data that LRL-CAT prides itself on. Both the software and hardware of the beamline is continuously being upgraded, a recent example of which is the installation of a Pilatus3 S 6M detector. In the past ten years, LRL-CAT has screened 119,447 crystals and collected 37,739 datasets, including 21,426 crystals and 6,714 datasets screened and collected for general users, respectively. Data collected at LRL-CAT has resulted in publications with many high-impact journals, such as *Nature*, *Journal of American Chemical Society*, and *Cell*. With a median turnaround of 25 hours (which includes ~16 hours of overnight shipping) from crystal harvest to processed data, LRL-CAT remains one of the most efficient beamlines in the world.

A-2

Improvements in Serial Crystallography Capabilities at GM/CA

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Successful proof-of-concept experiments have demonstrated the feasibility of synchrotron serial crystallography [1]. Recent hardware and software upgrades at GM/CA will allow routine user operation of serial data collection. Beam shape and intensity have been improved by the addition of compound refraction lenses (CRL). The CRLs provide nearly 10 times higher photon flux than the proof-of-concept measurements. All the components for high-viscosity injector-based sample delivery are installed in the ID-D endstation. During injector-based experiments, longer beam collimators and a tapered beam stop can be used to decrease background noise from air scatter before and after the sample. Fixed samples can generate serial datasets as well using a modified raster scan that allows sample rotation. The software suites Cheetah and CrystFEL as well as in house software allow real-time monitoring, data reduction, and processing.

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A-3

Ligand Exchange Method for High-throughput Crystallization of Novel Ligand-GPCR Complexes

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Rational structure-based drug design relies on the prior knowledge of the ligand binding mode to direct lead optimization. High-throughput structure determination methods of protein-ligand complexes is indispensable for tackling complicated problems giving a direct insight into receptor-small molecule interactions. We present a method for rapid, high-throughput and easy determination of structures of G protein-coupled receptors with various ligands to identify binding modes of those molecules.

Ligand exchange experiments were performed with A_{2A} and β2AR receptors. The structures revealed significantly strong omit electron density map for unambiguous identification of bound ligands. In addition, structures of β2AR complexes with two novel ligands—biased agonist carvedilol and antagonist propranolol were solved. Recently, we applied this method towards solving the structures of A_{2A} and MT_1 structures with a number of new ligands.

This approach is scalable and allows to set crystallization trials for a large variety of ligands at the same time from the same sample of protein in LCP. Furthermore, it allows rapid identification of the ligand binding site and the interactions involved for a panel of ligands in a single experiment. Ligand exchange approach broadens the range of ligands that can be crystallized in complex with GPCRs. This approach is useful for high-throughput structure determination or for crystallization of GPCRs with ligands that cannot be used directly for co-purification with the protein.

A-4

Investigating the Effect of Cholesterol on Supported Lipid Bilayers of Dipalmitoylphosphatidylcholine

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Integral membrane proteins are important constituents of biological membranes that play vital roles in a number of physiological processes such as cell signaling, cell-to-cell adhesion, signal transduction, and the transport of solutes across the membrane bilayer. One example, and our main interest, is lens-specific aquaporin-0 which is believed to maintain water homeostasis in the ocular lens which is required for lens transparency and elasticity. Evidence has emerged that the function of members of the aquaporin family of proteins, including aquaporin-0, depends on its lipid bilayer environment. Theoretical studies have provided insight into aquaporin-0/lipid bilayer structure but it is often difficult to gather experimental data on these systems.

A unique aspect of ocular cell membranes is their extremely high cholesterol content. In order to specifically understand the role of cholesterol on the ocular membrane interactions with aquaporin-0, we are developing methodology to prepare aquaporin-0/biomimetic membrane complexes and probe the structure of the complex with x-ray scattering, light scattering, and microscopy techniques. To that end, we have investigated the effect of cholesterol on supported bilayers of dipalmitoylphosphatidylcholine using x-ray reflectivity. Supported lipid bilayers were prepared from liposome formulations via a vesicle bursting method onto a silicon substrate and x-ray reflectivity data were collected at beam line 33-BM-C.

Obtaining unique, and physically meaningful fits to specular reflectivity data from multi-component membranes can be challenging. To address this problem, we have developed a new fitting methodology which parameterizes the membrane structure in terms of chemically meaningful parameters, rather than an arbitrary set of slabs. Molecular area, bilayer thickness, and cholesterol position were used as parameters in the fits. Phase diagrams of these parameters agree reasonably well with reported phase diagrams on these systems determined from NMR and DSC studies. Overall, this work provides us with necessary background information to ultimately better understand the aquaporin-0/lipid bilayer complex.

We would like to express our thanks to the Advanced Photon Source for granting us the time for these studies. We would like to express a special thanks to our beamline scientist, Jenia Karapetrova, for all her help in the experimental set-up at the beam line and training me to run the experiment.

Chemistry

A-5

New Pathways in Iron-based Water Oxidation Catalysis

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Solar energy has enormous potential as a clean, abundant, and economical energy source that can be captured and converted into useful forms of energy [1]. Hydrogen fuel can be obtained through splitting water and it is an optimal energy carrier for long term energy storage. This process of water oxidation requires a four electrons transfer process coupled to the removal of four protons from two water molecules and the formation of the oxygen-oxygen bond. The oxygen bond formation is considered as the main obstacle to achieve the overall water splitting. In order for this process to have a positive impact on the energy sector the catalyst material must be earth abundant. Here we study Fe-based water oxidation catalysts. Fe K-edge XANES were taken for effective water oxidation catalysts: initial $[Fe^{II}(mcp)(OSO_2CF_3)_2]$ and $[Fe^{II}(pytacn)(OSO_2CF_3)_2]$ powders and their solutions in HNO_3 oxidized with excess of Ce^{IV} or $NaIO_4$ [2]. Large shifts of the Fe K-edge position were observed for both compounds indicating formation of the Fe^{IV} and Fe^{V} species. Significant difference in oxidation behavior for these two complexes was discovered. Thus, Fe(mcp) complex displays Fe K-edge which is more consistent with overall Fe^{IV} oxidation state whereas oxidized Fe(pytacn) system shows formation of $[Fe^{V}=O(OH)(pytacn)]^{2+}$. EXAFS data obtained for products of [Fe(pytacn)] oxidation with Ce^{IV} or $NaIO_4$ are essentially identical and contain $Fe^{V}=O$ at ~1.60 Å.

Oxidation of $[Fe^{II}(mcp)(OSO_2CF_3)_2]$ lead to distinct products. Oxidation with periodate resulted in the shift of the first EXAFS peak to lower apparent distance which indicates formation of the short $Fe^{IV}=O$ bond. This elongation of the Fe=O distance relative to ~1.60 Å found for $Fe^{V}=O$ is in good agreement with the XANES data indicating Fe^{IV} oxidation state. Interestingly, oxidation with Ce^{IV}, while resulting in the same Fe^{IV} oxidation state, results in EXAFS with different spectral features. First peak in

the [Fe(mcp)] oxidized with Ce^{IV} is not shifted to shorter distance indicating lack of Fe=O interaction in this sample. Fe-O distance is consistent with bridging Fe-O-Fe unit. Relatively short Fe-Fe distance is consistent with di-μ-oxo bridged Fe^{IV}-O-Fe^{IV} unit. Complexes with highly oxidized Fe centers connected with di-μ-oxo bridges are very rare. The presence of the two Fe^{IV} centers makes Fe-Fe distance shorter 2.58 Å than 2.68 Å reported for Fe^{IV}-Fe^{III} di-μ-oxo complex. While no spectroscopic signatures of the peroxo intermediates have been noted our data do not contradict the possibility of the water nucleophilic attack on the $[(pytacn)Fe^{V}=O(OH)]^{2+}$ as the mechanism of the O-O bond formation.

We gratefully thank Argonne National Laboratory and 20-ID-B beamline staff for making this research possible.

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A-6

High Energy SAXS-WAXS Studies on the Fluid Structure of Molten LiCl-Li Solutions

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Molten mixtures of lithium chloride and metallic lithium (LiCl-Li) play an essential role in the electrolytic reduction of various metal oxides. These mixtures possess unique high temperature physical and chemical properties that have been researched for decades. However, due to their extreme chemical reactivity, no study to date has been capable of definitively proving the basic physical nature of Li dissolution in molten LiCl. In this study, the evolution of structures of the molten LiCl-Li, as metallic Li is electrochemically introduced into the melt, is investigated *in situ* with synchrotron radiation based high energy wide angle x-ray scattering (WAXS) and small-angle x-ray scattering (SAXS). The scattering results indicate the formation of Cl^- ion "cages" with size of approximately 7.9Å, which suggests the formation of Li clusters as previous reported. The pair distribution functions (PDF) of the melt derived from the diffraction results are in agreement with the ab-initio molecular dynamics simulation results. A physical model based on the formation and suspension of metallic Li cluster in lithium chloride is proposed to explain various phenomena exhibited by these solutions that were previously unexplainable.

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A-7

Understanding X-ray Spectroscopic Signatures of Photosystem II Using Mn Coordination Complexes

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Carbon based energy produced by single cellular organisms and plants is essential for the viability of almost all life on earth. Central to this process is water splitting, a four electron removal process which is initiated by photon absorption. In plants, a Mn_4O_XCa cluster, known as the oxygen evolving complex (OEC), and its surrounding ligand environment is used to store energy as it splits two waters and emits O2 in a cyclic process. This process consist of different semi-stable states, S0-S3, that advance upon light exposure. As each of these advance the Mn atoms in the OEC can change in oxidation state, ligand environment and geometry. This convolution of effects can make it difficult to understand the changes that occur throughout each state transition. While the oxidation state of most states is well known through x-ray spectroscopic measurements, the S3 state remains elusive due to controversial findings in EPR, XAS and XES. While EPR [1], XAS and XES [2] were initially interpreted as though Mn was not oxidized during the S2-S3 transitions, this assessment has since been revisited. While it has been suggested that x-ray spectroscopy could be affected by competing effects, hypothesized to be simultaneous coordination number and oxidation state changes, which result in weak shift towards oxidation, this has not been systematically supported. Here we examine a series of Mn compounds to compare changes in ligand coordination number and examine the resultant effects. We examine the changes of 5 and 6 coordinated Mn compounds that are the same in the first coordination sphere and compare the magnitude of the spectral shifts in Mn to that obtained with PSII. The results are discussed in context of the OEC and plausible changes throughout the cycle.

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A-8

Breakage and Restructuring of Boehmite Aggregates Analyzed by *in situ* Capillary Rheometry, Ultra-small Angle, Small Angle, and Wide Angle X-ray Scattering

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The U.S. government plans to remediate 56 million gallons of mixed radioactive and chemical waste stored in 177 underground tanks at the Hanford Site in Washington, USA. Sludges in the tanks are sparingly soluble and will be removed as slurries per the current remediation plans. The aqueous component of the slurries is highly alkaline and contains high concentrations of electrolytes. Despite being as small as nanometer in size, the particulates have a propensity to aggregate in these streams, heavily influencing the process stream rheology during treatment [1].

A key challenge for developing tank waste processing schemes is modeling the behavior of sludge suspensions as a function of changing chemical and physical conditions. These include electrolyte composition and concentrations, temperature, and flow rates. Such predictive models are based on knowledge of interactions between particles, as manifested by slurry rheology. However, classical approaches to colloidal dispersions do not provide sufficient consideration of structural anisotropy under the extreme chemical conditions that are encountered during the processing of highly radioactive wastes [2].

Recent studies have begun investigating the aggregation behavior of boehmite [γ-AlO(OH)], one of the major crystalline phases identified in the Hanford waste sludges, at elevated ionic strengths and pH values [3]. In this study, capillary rheometry and in-situ wide, small, and ultra-small angle x-ray scattering (WAXS, SAXS, USAXS) have been combined to quantify changes in viscosity, aggregation, breakage, and restructuring as a function of flow conditions. In addition, computational fluid dynamics (CFD) has been used to rigorously characterize the fluid flow, providing a basis for modeling the viscosity as a function of forces between particles, stability, and aggregation/breakage. This study will serve as a benchmark to compare with future work in which additional chemical complexity (e.g., elevated ionic strength) will be introduced.

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A-9

Tracing Ion Concentrations in Back-extraction Processes via X-ray Fluorescence near Total Reflection

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Solvent extraction processes are under development to optimize the efficiency and kinetics of the separation and recovery of lanthanides and actinides in nuclear fuel cycles. Forward and backward extraction processes rely upon the transfer of metal ions across the liquid-liquid aqueous-organic interface. Although the interaction of metal ions with aqueous complexants, buffers, and organic extractants at the aqueous-organic interface is likely to determine the efficiency and kinetics of extraction processes, little is known about how complexing molecules and metal ions organize at the interface or the mechanism of ion transport across the interface.

Here, we present preliminary data from first experiments whose purpose is to characterize the presence of ions at the interface under conditions relevant to back-extraction in the ALSEP process. A liquid organic phase containing Eu-extractant complexes is placed into contact with an aqueous phase containing citric or nitric acid. X-ray fluorescence near total reflection (XFNTR) is then used to measure the ion concentration at the interface and in the two bulk phases. These measurements reveal that the citric acid solution back-extracts the Eu ion more efficiently than the nitric acid solution, though the latter stabilizes Eu ions at the interface. In addition, XFNTR data analysis that distinguishes fluorescence signals from ions in three different locations (the bulk aqueous phase, the bulk organic phase, and the interface) will be described.

A-10
Surface Sensitive Spectroscopy for Understanding Liquid-liquid Extraction

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The increase in global population strains supply of clean water and puts high demands on the energy capacity. Central to meeting these environmental and economic challenges is innovation and implementation of advanced separation technologies. In particular, liquid-liquid extraction of the f-block elements is important for metal refining and nuclear waste treatment. During extraction, an amphiphilic surfactant is used to transfer the metal ions from an aqueous environment to an organic phase. The acidity of the aqueous phase, the presence of counter ions, and the surfactant are all important parameters determining the efficiency and selectivity of the extraction process. Due to the complexity and breadth of the problem space, knowledge of the molecular interactions affecting extraction is extremely limited and there is little predictive insight for designing new systems. As the extracted species must pass through an interfacial boundary during extraction, monitoring and understanding the interface between the extractant and aqueous phase can help unravel important questions in the field. Surface specific x-ray scattering and fluorescence are the most direct ways to probe liquid surface and interface structures. Sum frequency generation (SFG) spectroscopy is another surface sensitive technique that gives vibrational information of species at the surface. SFG is frequently used to study hydrogen bonding networks at charged and neutral surfaces and provides molecular detail complementary to the information provided by x-ray techniques. Here I discuss the SFG spectroscopic technique and provide an example of the complementary application of x-ray fluorescence and SFG to understand the disparate effects of ions at the water/surfactant interface.

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A-11
X-ray Absorption Spectroscopy for Single-atom Catalysts at 9-BM

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Single atom catalysts (SACs), offering maximized atom-use efficiency and unique coordination environments, are of great interests for catalytic activity and/or selectivity enhancements for many reactions including oxidation, hydrogenation, electro-catalysis, and so on. In general, atomic dispersions can be achieved in wet chemical synthesis by the confinement and coordination of metal atoms to the substrate and prevent such aggregation at mild temperatures. Recent studies have sought to improve the thermal stability of single atoms by enhancing the metal-substrate absorption using kinetic or spatial confinement or forming strong metal-substrate bonds by annealing at 800–900°C.

X-ray absorption spectroscopy (XAS) is a powerful technique to determine geometric and electronic structure of active sites in catalysts. XAS contains x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS). XANES is typically used to determine the oxidation state of the probed atom and EXAFS for the local coordination environment. With the EXAFS, the atomic dispersion of the SACs can be verified. The bond distance and coordination numbers around the active atom in the SACs can be experimentally determined to understand the mechanism of the SACs. The undercoordinated single-atom sites and their mechanisms have been identified for several SAC systems by XAS at 9-BM.

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[1] *Adv. Energy Mater.* (2019) **9**: 1803737.

A-12

Synchrotron Hard X-ray Spectroscopic Investigation of the Photoaquation Reaction Mechanism in Hexacyanoferrate(II) with Sub-pulse Temporal Resolution

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Synchrotron hard x-ray sources, such as the Advanced Photon Source (APS), provide high-repetition-rate, ultra-stable, widely tunable x-ray pulses with average flux comparable to that of XFELs. These characteristics allow for precision spectroscopic measurements with elemental selectivity, of systems in complex environments. Leveraging rapid advances in ultrafast optical laser technology, we have built a liquid-jet endstation at the APS that fully utilizes the x-ray flux for laser-pump, x-ray-probe measurements. While it is often assumed that the temporal resolution of such measurements is limited by the x-ray pulse duration to timescales ~100 ps and longer, we show that by incorporating the so-called “time-slicing” technique, where a short-duration laser pumps the sample within the temporal envelope of the probing x-rays, the spectroscopic properties of short-lived species can be investigated with sub-pulse-duration time resolution. Using this method, we explored the photo-induced ligand substitution reaction of $[Fe(CN)_6]^{4-}$ in aqueous solution, capturing the spectrum of the penta-coordinated intermediate and determining its lifetime to be ~15 ps. Comparison with QM/MM calculations provides elucidation of the aquation mechanism.

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A-13

In situ Experiments Using Synchrotron Techniques

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Heterogeneous catalysis is one of the most important branches of applied chemistry. Nowadays, most of the industrial products (from chemicals to energy) require the use of catalysts at some point during the process. Catalysts studies are difficult due to their properties; they are unstable, highly reactive and constantly change depending on the environments, such as temperature, pressure, humidity, chemicals, etc. As the structural and electronic properties under reaction conditions are of great importance to elucidate the reaction mechanism, the study of the catalyst under real operating conditions is crucial. Only after, a rational design can enhance their properties. To achieve this goal, *in situ* or *operando* characterization experiments are very important and very common nowadays.

In this work, we will present several capabilities that are ready to perform *in situ* experiments in the Spectroscopy Group at APS Sector 20. Some research examples will be shown to illustrate the kind of information that can be achieved with these techniques and the sample environments that are available to general users. Special attention will be given for some recent results obtained for single atoms catalysts. The electronic properties of atomically dispersed catalysts are different from their bulk and nanoparticles counterparts leading to different active sites and potential new applications. In this example, we will show the different properties of single atoms catalysts prepared using different supports. We will show valuable information that can be obtained only performing in situ experiments and can help to explain how the metal-support interaction can influence stability and reactivity of these materials.

This research used resources 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, and the Canadian Light Source and its funding partners.

A-14

Structural Analysis in Soft Matter Using Synchrotron X-ray Scattering Techniques

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Here we describe the application of synchrotron based x-ray scattering techniques to analyze the structure of two related soft matter systems: assemblies of nanoparticles, and reverse micelles formed in solvent extraction systems. Using small angle x-ray scattering (SAXS) and x-ray reflectivity, we demonstrate that nanoparticles functionalized with polyelectrolytes self-assemble into 2D and 3D ordered structures, primarily driven by hydrogen bonding between neighboring polymer chains, similar to programmable assembly using complementary DNA strands [1,2]. We functionalize gold nanoparticles (AuNPs) with poly(acrylic acid)-thiol (PAA-SH) to form a AuNP-PAA core-shell nanoparticles and bridge neighboring nanoparticles via inter-chain hydrogen bonding between protonated poly(acrylic acid) chains in the shell. Monolayers of AuNP-PAA form at the air-water interface, while nanoparticle aggregates with short-range order are formed in the bulk solution. We show the effect of pH and length of PAA chains on the inter-particle distances in the assemblies. Implications of these results in the context of inter-polymer complex mediated assemblies [3,4] will be discussed. Using simpler synthetic polymers instead of DNA allows easier processing and facile implementation of block copolymer based self-assembly techniques.

Similar to the hydrogen-bond driven assembly of nanoparticles described above, it is hypothesized that the non-covalent interactions between reverse micelles in solvent extraction systems affect the extraction behaviors such as extraction efficiency and the formation of the third phase [5]. We will discuss some preliminary SAXS results with lanthanide-bearing reverse micelles in organic solvents.

Nanoparticle self-assembly work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at the Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358. Solvent extraction studies are supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Chemical Sciences, Geosciences, and Biosciences, under Contract No. DE-AC02-06CH11357. 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, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

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A-15

Amidoxime-functionalized Ultra-high Porosity Materials for ^{230}Th and ^{233}U Separations

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The leaching of early actinides including U and Th as well as other fission products into groundwater remains a critical human health and environmental issue. Strategies for removal of radionuclide contaminants often involve batch processes such as solvent extraction. Taking advantage of new advancements in adsorbent materials as an alternate strategy to contaminant removal, we present the development of an understudied class of actinide adsorbents with the potential to meet these challenges. Polymerized high internal phase emulsions (poly(HIPEs)) are hierarchically porous polymer monoliths with pore diameters on the order of 500 nm whose synthesis can easily be tailored to allow incorporation of functional monomers. Nitrile containing polystyrene-based poly(HIPEs) have been prepared through the use of either acrylonitrile (AN) or 4-cyanostyrene (4CS) comonomers. Post-synthetic modification of these nitrile-containing poly(HIPEs) renders their corresponding amidoximated analogues which were studied for actinide uptake.

These amidoxime-functionalized porous monoliths were shown to adsorb 95% ^{230}Th from aqueous solution within 30 minutes. Uptake of ^{233}U is lower under similar

conditions, with selectivity factors (α) over ^{233}U of ~100. Preliminary uptake data suggest a different binding mechanism for Th vs. U under the same conditions and is currently under investigation. Due to their high affinity for Th as well as inherently porous structure, these materials may find use in continuous flow processes for water purification. By combining radiotracer and bulk metal analysis a more complete assessment of material performance across a broad range of metal concentrations has been achieved.

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A-16

Micro-focused MHz Pink Beam for Time-resolved X-ray Emission Spectroscopy

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X-ray emission spectra (XES) in the valence-to-core (vtc) region offer direct information on occupied valence orbitals. They emerge as a powerful tool for the ligand identification, bond length, and structural characterization. However, the vtc feature is typically two orders of magnitude weaker than K alpha emission lines, making it hard to collect, especially for transient species. To overcome the difficulty, pink beam excitation capability was demonstrated recently at Sector 7 of the Advanced Photon Source. A water-cooled at mirror rejects higher harmonics, and beryllium compound refractive lenses (CRLs) focus the reflected fundamental beam (pink beam) to a 40μm × 12μm elliptical spot at sample target that matches the laser spot size used for photoexcitation. With an x-ray flux of 10^15 photons per second, non-resonant XES spectra were taken on iron(II) hexacyanide and on photoexcited iron(II) tris(2, 2'-bipyridine). We could reproduce previous measurements with only a fraction of the acquisition time, demonstrating the ability to measure high quality spectra of low concentration species.

Work was supported by the U.S. Department of Energy, Office of Science, Chemical Sciences, Geosciences, and Biosciences Division.

A-17

Probing Open Metal Sites in High Valence Metal-organic Frameworks by *in situ* Single Crystal X-ray Diffraction

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The crystallographic characterization of framework–guest interactions in metal–organic frameworks enables the location of guest binding sites and provides meaningful information on the nature of these interactions, allowing the correlation of structure with adsorption behavior. Herein, techniques developed for in situ single-crystal x-ray diffraction experiments on porous crystals have enabled the direct observation of CO_2 adsorption in the open metal site of $Fe_{3-x}M_xO$ clusters (X=0, 1, 2) in PCN-250. PCN-250 is a metal–organic framework that can possess trivalent and bivalent metals in the cluster [1]. The single crystal samples were characterized before and after activation in N_2 at 423 K and after CO_2 adsorption. Interestingly, the CO_2 binding is stronger to the bivalent metals than to the trivalent metals, indicating orbital interaction plays a bigger role in the gas-open metal site interaction than the static electric force. To the best of our knowledge, this work is the first single-crystal structure determination of a trivalent metal–CO_2 interaction and the first crystallographically characterized open metal site for trivalent metals.

We acknowledge the support from the Advanced Photo Source on beamline 15ID-B of ChemMatCARS Sector 15.

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A-18

Investigations of Catalysis and Batteries at Beamline 9-BM: Capabilities and Upgrade

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As a beamline dedicated to the x-ray absorption spectroscopy (XAS), 9-BM is capable to cover very wide energy range (2145.5 eV P-K edge to 24350 eV Pd-K edge). In recent years, more efforts have been devoted to the fields of catalysis and energy storage, focusing on catalysis for efficient conversion of energy resources into usable forms, and storage of such energy in efficient and safe capacitors. To understand and predict

how catalysts and/or energy storage materials function, it is very important to characterize the materials under actual reaction conditions (*in situ* or *operando*). 9-BM has leveraged the advanced capabilities for *in situ* catalysis and electrochemistry, as well as the ability to collect high quality spectroscopy data at a rapid rate (Quick EXAFS). Scientists using 9-BM are able to gain unique insight to how chemical processes affect and are affected by the materials under investigation.

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, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

Environmental Science and Geology

A-19

Understanding the Morphological Evolution in CO_2-responsive Nanofluids during the Hydrogel Formation Using Time-resolved USAXS/SAXS Measurements

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The development of CO_2 based fracturing for enhanced subsurface energy recovery has gained significant importance, recently. However, the delivery of proppants to enhance the permeability by keeping the pore spaces open in CO_2 based fracturing is still a challenge. In this study, we propose CO_2-responsive nanofluids constructed from SiO_2 nanoparticles and poly(allylamine) (PAA), which form hydrogel on reaction with CO_2. Time resolved USAXS/SAXS measurements were performed to understand the aggregate formation during CO_2 loading and hydrogel formation. Further, Gaussian coil-like morphology was noted on CO_2 loading. Accelerated hydrogel formation in these nanofluids was directly related to enhanced CO_2 absorption capacity compared to the pure polymer precursors. Fourier-Transform Infrared Spectroscopy (FT-IR) measurements showed the formation of carbamate, protonated primary and secondary, and bicarbonate ions in CO_2-loaded pure polymer, PAA and SiO_2-PAA nanofluids. These studies suggest that the morphological changes leading to hydrogel formation are facilitated by CO_2-induced chemical changes.

A-20

Identifying Poultry Litter Ash Phosphorus Speciation and Submicron Structure Composition Effect on Efficiency as a Maize Fertilizer

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As the expanding world population places pressure on the poultry industry to meet consumption demands, heightened poultry litter (PL) production presents an obstacle to identify alternative uses for increased volumes. Repeated PL applications within localized distances of poultry operations creates nutrient concentrated areas posing a threat to Cheaspeake Bay ecosystems. Poultry litter ash (PLA), a co-product from manure-to-energy systems, is a promising solution addressing: transportation logistics, repurposing PL nutrients, and offers dual purpose as a fertilizer and a green energy source. The objective of this study is to characterize PLA speciation, elemental composition, and P solubility. Therefore, the first objective is to determine phosphours (P) speciation in four PLA fertilizers: Fluidized Bed Bulk, Combustion Mix, Fluidized Bed Fly Ash, and Granulated Poultry Litter Ash via XANES spectroscopy.

Additionally submicron amorphous and crystalline structures were identified through back scatter electron micrsocopy to identify qualtative elemental composition. Accompanying spectroscopy and miscroscopy techniques, a total elemental analysis, water soluble P, and sequential extraction experiment were conducted to elucidate nutrient availability and solubility. Thermo-conversion systems high temperatures (~593 C) alter PLA nutrient solubility; therefore, phosphorus fertilizer sources were extracted sequentially using deionized water, $NaHCO_3$, NaOH, HCl and finally acid digested using EPA 3050B followed by analysis via ICP-AES. Water extraction represented soluble P (Sp%) whereas $NaHCO_3$ signified labile inorganic P (Lp%). Phosphorus extracted by NaOH, HCl, EPA 3050B acid digestion reflects non-labile or bound plant unavailable P (Bp%). Characterizing PLA elemental and chemical composition is imperative to validate PLA coproducts as a comparable fertilizer source and subsequently calibrate fertilizer recommendations for crop application. Determining PLA fertilizer elemental composition is a foundational component validating PLA as an alternative P fertilizer source and subsequently promoting surplus nutrient redistribution from concentrated poultry production regions to nutrient deficient areas within the USA.

A-21

The Role of Nano-interface of Hemoilmenite in Enhancing Remanent Magnetization

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Hematite–ilmenite (Fe_2O_3-$FeTiO_3$) series have strong remanent magnetization, suggesting an explanation for some magnetic anomalies from igneous and metamorphic rocks in the Earth's crust and even Martian crust. The problem is that the unusual remanent magnetization cannot be explained by the properties of individual magnetic minerals such as hematite and ilmenite. Previous studies have attributed the strong remanent magnetic property to fine exsolution lamellae related to local redox conditions and cooling history of rock [1]. However, the exact role of exsolution lamellae in enhancing magnetic stability is still not clear. We aim to determine the structure and chemistry of nano-scaled hematite and ilmenite exsolution lamellae, which correlated with the magnetic properties. Here, we present the preliminary results of the interface structure of hemoilmenite exsolution using the nano-scaled elemental mapping from FEI Talos F200X TEM/STEM (CNM) and high-resolution XRD (11-BM, APS). The results show that the size and interface structure of exsolution lamellae plays an essential role in enhancing the strong remanent magnetization of hemoilmenite and provide an explanation for coercivity and strong remanent magnetization in igneous, metamorphic rocks and even some reported Martian rocks. These nano-scaled interfaces and structures could extend our knowledge of magnetism and help us to understand the diverse magnetic anomalies occurring on Earth and other planetary bodies.

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A-22

Iodine Immobilization by Silver-impregnated Granular Activated Carbon in Cementitious Systems

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^{129}I is a major long-lived fission product generated during nuclear power generation and nuclear weapon development. Over the years, ^{129}I has been inadvertently introduced into the environment from leaks at waste storage facilities and currently is key risk driver at the U.S. Department of Energy (DOE) sites. The most common chemical forms of I in liquid nuclear wastes and in the environment are iodide (I^-), iodate (IO_3^-) and organo-I. They display limited adsorption onto common sediment mineral, are highly mobile and difficult to be immobilized. As the stockpile of ^{129}I-bearing nuclear waste continues to increase rapidly, novel sequestration technologies are needed to reduce its potential contamination of the environmental and living organisms.

Silver (Ag)-based technologies are amongst the most common approaches to removing radioiodine from aqueous waste streams. As a result, a large worldwide inventory of radioactive AgI waste presently exits, which must be stabilized for final disposition. In this work, the efficacy of silver-impregnated granular activated carbon (Ag-GAC) to remove I^-, IO_3^- and organo-I from cementitious leachate was examined. In addition, cementitious materials containing I^-, IO_3^-, or organo-I loaded Ag-GAC were characterized by iodine K-edge XANES and EXAFS using the beamline 10-BM at the Advanced Photon Source (APS) to provide insight into iodine stability and speciation in these waste forms. The Ag-GAC was very effective at removing I^- and organo-I, but ineffective at removing IO_3^- from slag-free grout leachate under oxic conditions. I^- or organo-I removal was due to the formation of insoluble AgI(s) or Ag-organo-I(s) on the Ag-GAC. When I^- loaded Ag-GAC material was cured with slag-free and slag grouts, I^- was released from AgI(s) to form a hydrated I^- species. Conversely, when organo-I loaded Ag-GAC material was cured in the two grout formulations, no change was observed in the iodine speciation, indicating the organo-I species remained bound to the Ag. Because little IO_3^- was bound to the Ag-GAC, it was not detectable in the grout.

Thus, grout formulation and I speciation in the waste stream can significantly influence the effectiveness of the

long-term disposal of radioiodine associated with Ag-GAC in grout waste forms. This study also has implications on appropriate subsurface disposal sites. For example, some proposed disposal sites under consideration were selected in part because they possess naturally reducing system. Reducing conditions are expected to reduce the mobility of some key aqueous radionuclides that are redox-sensitive, most notably Np, Tc, Pu, and U. However, such reducing systems may exacerbate safe disposal of I^- loaded Ag-GAC secondary solid waste.

A-23

Understanding P Dynamics of Delmarva Peninsula "Legacy" P Soils by X-ray Absorption Near Edge Structure Spectroscopy (XANES)

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Past application of phopshorus (P) fertilizers and poultry manures exceeding crop uptake resulted in P-saturated soils on the Delmarva Peninsula, a large peninsula in the mid-Atlantic containing Delaware and portions of Maryland and Virginia. Numerous artificial drainage ditches act as conduits for excess P to waterways such as the Chesapeake Bay, resulting in eutrophication and hypoxia. With increased regulations on fertilizers and manure application, Delmarva farmers are finding managing this historically applied "legacy" P and providing enough available P for crop growth to be difficult. The goal of this project is to investigate P dynamics in legacy P soils using chemical extractions (e.g., Hedley extractions) and advanced spectroscopic tools. To identify the dominant chemical forms of P present in the soil, we used x-ray absorption near edge structure spectroscopy (XANES) at the bending magnet beamline (9-BM) of the Advanced Photon Source, Argonne National Laboratory. Our preliminary XANES fitting results indicated that the predominant forms of P included PO(4) sorbed to Al hydroxides, phosphosiderite, and strengite. Further XANES spectra conducted on legacy P soils paired with chemical extractants will help unravel the nature of P in manure and fertilizer impacted legacy P soils on the Delmarva, leading to better P management decisions and improved water quality.

High Pressure

A-24

Single-crystal X-ray Diffraction at Extreme Conditions

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The advantages of using single crystals over powdered samples in x-ray diffraction experiments are well known [1]. Analysis of single-crystal x-ray diffraction (SCXRD) data has traditionally allowed us to obtain explicit solutions of complex structures, detect small structural distortions, retrieve accurate displacement parameters as well as provide chemical characterization of new materials. The SCXRD method is becoming more and more appealing in the high-pressure research community nowadays [2]. It is now possible to study in great details the crystal structure, physical and chemical properties of minerals and materials, important for materials science, even in the megabar pressure range using the diamond anvil cell (DAC) [3]. Even at high pressure, where the coverage of the reciprocal space is restricted by the DAC design, SCXRD data provide more information than the one-dimensional diffraction patterns collected from powdered samples.

Here we review the sample and DAC preparations that are necessary prior to a single-crystal x-ray diffraction experiment, we describe the data collection procedures at GSECARS beamline (sector 13), and we discuss the data processing using various software. A few examples on carbonate minerals and various metal oxides are presented in order to demonstrate not only the challenges but also the advantages of using single crystals for solving the structures of complex high-pressure polymorphs or novel compounds, as well as to better constrain the compressibility and the high-pressure structural evolution of known compounds.

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Instrumentation

A-25

Recent Developments in BIO-SAXS Using MetalJet X-ray Source

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High-end x-ray scattering techniques such as SAXS, BIO-SAXS, non-ambient SAXS and GISAXS rely heavily on the x-ray source brightness for resolution and exposure time. Traditional solid or rotating anode x-ray tubes are typically limited in brightness by when the e-beam power density melts the anode. The liquid-metal-jet technology has overcome this limitation by using an anode that is already in the molten state. With bright compact sources, time resolved studies could be achieved even in the home laboratory. We report brightness of 6.5×10^{10} photons/(s mm^2·mrad^2·line) over a spot size of 10 µm FWHM.

Over the last years, the liquid-metal-jet technology has developed from prototypes into fully operational and stable x-ray tubes running in more than 8 labs over the world. Multiple users and system manufacturers have been now routinely using the metal-jet anode x-ray source in high-end SAXS set-ups. With the high brightness from the liquid-metal-jet x-ray source, novel techniques that was only possible at synchrotron before can now also be used in the home lab. Examples involving in-situ measurements and time resolution such as SEC-SAXS or growth kinetics with temporal resolution on the order of seconds will be shown.

This presentation will review the current status of the metal-jet technology specifically in terms of stability, lifetime, flux and optics. It will furthermore refer to some recent SEC-SAXS and bio-SAXS data from users.

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A-26

Commissioning of XTIP Beamline at the Advanced Photon Source

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We present a report on the ongoing XTIP beamline construction project at the Advanced Photon Source (APS) for a state-of-the-art synchrotron x-ray scanning electron microscopy (SX-STM) system. When completed, the beam line will provide highly collimated monochromatic x-ray beam from 500 to 2400 eV energy range, and that will be used for advanced nanoscale probing of the chemical, electronic and magnetic properties. The beamline currently consists of three mirrors, M1–M3, a spherical grating monochromator (SGM), two slits—entrance and exit, a sample stage and is maintained at ultra-high vacuum (UHV) using a combination of turbomolecular and ion pumps at different stages. The insertion device selects an x-ray energy range which is further narrowed down and focused by M3 unto the SGM. The entrance and exit slits control the beam intensity upstream and downstream respectively, while the SGM produces a monochromatic beam from the incoming broad spectrum that goes into the sample stage. The sample stage holds a metal tantalum, single-crystal silicon and germanium and indium-phosphor samples which are used for beam optimization and calibration of the monochromator. So far, we have been able to focus a coherent, monochromatic beam unto these samples and obtain their x-ray absorption spectroscopy which are in good agreement with known standards. The next phase of the project involves the installation of two focusing mirrors, M4 and M5, mounting of the UHV optical beam chopper, further beam optimization and SGM energy calibration and the integration of the fully operational beamline with the STM, which is also currently under construction at the end station.

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A-27

Status of the Diamond CRL Development

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The next generation light sources such as diffraction-limited storage rings and high repetition rate free electron lasers (FELs) will generate x-ray beams with significantly increased peak and average brilliance. These future facilities will require x-ray optical components capable of handling large instantaneous and average power densities while tailoring the properties of the x-ray beams for a variety of scientific experiments.

Euclid Techlabs had been developing x-ray refractive lens for 3 years. Standard deviation of lens residual gradually was decreased to sub-micron values. Post-ablation polishing procedure yields ~10 nm surface roughness. In this paper we will report on recent developments towards beamline-ready lens. This will include recent measurements at the Advanced Photon Source.

A-28

Mega-electron Volt *Lab-in-Gap* Time-resolved Microscope to Complement APS-U: Looking into Solid State Chemistry for Energy Applications

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A recent finding made at the Advanced Photon Source provided new insights into how an iron oxide reacts with diluted gastric acid (which is a basic inorganic high school reaction) [1]. The news said that reactions do not happen uniformly and instantaneously and that precursor shapes and morphologies can alter reaction kinetics. Now it is important to acknowledge—neither starting location of reaction nor reaction front and its spatial propagation, nor kinetics rates, nor intermediate products are known *a priori*. Add to this, various temperatures that can mediate even simple reactions differently. Similar irreversible processes evolve in any solid-state systems at short length and time scales, and the final products (converted from precursors to vast output amounts that have to be obtained in the right stoichiometry and crystal structure form) have tremendous importance in metallurgy, chemical engineering, microelectronics.

These are the perfect problems for synchrotrons as they can shoot through reaction zone to get insights, but it is challenging for synchrotrons to pinpoint fast process in *k*-space with high spatial resolution/localization. Electron microscopy is perfectly suitable for high spatial resolution/localization. Therefore, a high pass through (MeV) *Lab-in-Gap* time-resolved electron microscopy is proposed to complement APS-U for this kind of tasks. *Lab* stands for multi-modal (optical, thermal, mechanical, electrical, electrochemical, etc.) probing *in situ* and *in operando*, and could enable (i) quantitative measurements of materials structure, composition, and bonding evolution in technologically relevant environments; (ii) understanding of structure-functionality relationships. The proposed MeV *Lab-in-Gap* microscope takes advantage of a new tunnel and a high duty cycle gun at APS, and can address the most critical and outstanding questions related to sustainable and renewable energy production and storage [e.g., (i) cycled electro-chemical reactions in batteries and (ii) thermochemistry behind synthesis of earth abundant materials crucial for future photovoltaics].

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A-29

Ultrafast Hard X-ray Modulators Based on Photonic Micro-systems

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Time resolved x-ray studies at synchrotron facilities have been a productive approach to study the temporal and spatial evolution of material systems at the time scale of 100 picoseconds, the pulse length of x-rays. The latest development of ultra-bright x-ray sources, including the APS-U, will enhance the techniques with a much higher coherent x-ray flux. But since these new sources are often associated with high bunch repetition rates on the order of 100 MHz, they impose a challenge for x-ray optics and detectors to handle individual x-ray pulses. We demonstrate here a new set of x-ray photonic devices based on micro-electro-mechanical systems that can effectively manipulate hard x-ray pulses on a time scale down to 300 picoseconds, comparable to the pulse length of x-rays.

The devices operate in a diffraction geometry, where the millidegree-scale static Bragg peak of single-crystal silicon

resonators is converted to a nanosecond-scale diffractive time window as the resonators oscillate. The diffractive time window can be flexibly tuned from a few nanoseconds down to 300 picoseconds with the change of applied voltage or an adjustment of the ambient pressure. The short diffractive time window of these miniature devices brings unprecedented design capabilities for beamlines to manipulate x-ray pulses. We demonstrate that these devices can be applied as ultrafast x-ray modulators, picking single x-ray pulses from pulse trains at APS as well as from the 500 MHz pulse train at NSLS-II. Derived from this pulse-picking capability, the devices can also be used to diagnose an x-ray fill pattern by measuring the intensity of each individual x-ray bunch. Further optimization of devices foreshadows a feasible diffractive time window of 100 picoseconds and below and new capabilities of x-ray pulse streaking and pulse slicing. It thus will become possible to achieve a temporal resolution below the x-ray pulse-width limit without interfering with the storage-ring operation.

A-30

Advanced Spectroscopy and LERIX Beamlines at Sector 25 for APSU

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The programs at 20-ID will be moving to 25-ID to make room for a long beamline. In addition, the new beamlines will support the laser pump-probe spectroscopy programs at 7-ID and 11-ID. Thus, the new sector will have a canted undulator with two beamlines, the Advanced Spectroscopy and LERIX (ASL) beamlines. The canted undulator beams will be separated using side deflecting mirrors that can also provide some degree of horizontal focusing. The liquid nitrogen cooled monochromators will have a multilayer option for high-flux non-resonant spectroscopy. There will be three experimental hutches. The first experimental hutch will house a variable resolution microprobe with a large variety of detector options. This will be a side station with about 30 cm clearance from the second undulator beam. The back two experimental hutches will share the second beam and have multiple stations supporting an upgraded LERIX spectrometer, high resolution emission spectroscopy such as HERFD, and the laser pump-probe experiments. This poster will show the beamline layout, some optics details, and the progress to date. First beam is expected in the summer of 2020.

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A-31

A Comparison of Isolated and Monolithic Foundation Compliance and Angular Vibrations

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The *in situ* nanoprobe (ISN, 19-ID) beamline will be a new best-in-class long beamline to be constructed in a new satellite building as part of the Advanced Photon Source Upgrade (APS-U) project. A major feature of the ISN instrument will be the Kirkpatrick-Baez (K-B) mirror system, which will focus x-rays to a 20 nm spot size with a large working distance of 50 mm. Such a large working distance allows space for various in situ sample cells for x-ray fluorescence tomography and ptychographic 3D imaging. However, the combination of spot size, mirror size, and working distance requires a highly stable instrument, < 3 $nrad_{RMS}$ vibrations (1–2500 Hz) for the vertical focusing mirror. To achieve such a stable requirement, an ultra-low compliance foundation with angular vibrations less than the mirror requirement is needed. Two types of foundations have been proposed, a large monolithic foundation slab for the entire building, thickening to 1 m under the instrument, or an isolated 1 m thick instrument foundation slab. For comparison, measurements of the compliance and angular vibrations of the APS experiment floor (0.6 m thick section, monolithic) and the sub-angstrom microscopy and microanalysis (SAMM) building 216 at Argonne National Laboratory (1.0 m thick, isolated) were acquired. In addition, an analytical analysis of whether or not to place the concrete enclosure on the isolated instrument slab was conducted. It was found that the slab at SAMM had less compliance from 10–200 Hz than the APS floor slab. Angular vibrations from (5–500 Hz) of the SAMM slab were 2.6 $nrad_{RMS}$ and for the APS slab 4.6 $nrad_{RMS}$. Lastly, the analytical analysis showed that vertical and angular compliance was reduced when the concrete enclosure was placed on the isolated slab. In conclusion, a 1 m thick isolated slab out performs a monolithic slab while also benefitting from isolation of the surrounding cultural noise sources.

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A-32

Combined Scanning Near-field Optical and X-ray Diffraction Microscopy: A New Probe for Nanoscale Structure-property Characterization

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A new multimodal imaging platform has been developed at station 7-ID-C at the Advanced Photon Source, incorporating scattering-type scanning near-field optical and x-ray nanobeam diffraction microscopy. The correlative imaging capabilities available with the "XSNOM" allow the atomic structure and optical properties of electronic materials to be characterized under a variety of external stimuli, including applied electric field, temperature, and pressure. We demonstrate the new capabilities in structure-property characterization available with XSNOM by probing the insulator-to-metal transformation in vanadium dioxide thin films induced by an applied electric field and by heating through the critical temperature. We have also explored the defect-coupled local polarization switching behavior of Pb(Zr,Ti)O3 thin films, a model ferroelectric system, as electrically and mechanically induced by a scanning tip. The XSNOM instrument advances the state of microscopic materials characterization by enabling the simultaneous imaging of the crystal structure and functional properties combined with *in situ*, local manipulation of electronic materials.

This work was supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division. 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.

A-33

Development of Transition-edge Sensor X-ray Microcalorimeter Linear Array for Compton Profile Measurements and Energy Dispersive Diffraction

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X-ray transition-edge sensors (TESs) offer the highest energy resolution of any energy-dispersive detector: ~1 eV at 1 keV, ~3 eV at 6 keV and ~50 eV at 100 keV. We are currently building a TES x-ray spectrometer for the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) for energies less than 20 keV. The spectrometer consists of application specific TES sensors designed, fabricated, and tested at ANL. We propose to develop these TES sensors for the very hard x-ray energy range (20–100 keV) for energy-dispersive x-ray diffraction (EDXRD) and Compton scattering. We have recently published an article where we present a design optimization for a TES x-ray microcalorimeter array for EDXRD and Compton profile measurements [1]. We present our progress on simulation results, preliminary sensor layouts, and proof-of-principle fabrication of millimeter long SiN membranes.

This work was supported by the Accelerator and Detector R&D program in Basic Energy Sciences' Scientific User Facilities (SUF) Division at the Department of Energy. This research used resources of the Advanced Photon Source and Center for Nanoscale Materials, U.S. Department of Energy Office of Science User Facilities operated for the DOE Office of Science by the Argonne National Laboratory under Contract No. DE-AC02-06CH11357. The authors gratefully acknowledge assistance from CNM staff, especially D. Czaplewski and S. Miller.

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A-34
(The) RAVEN at 2-ID-D

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Once upon a late beamtime dreary, the beamline scientist pondered, tired, weak, and weary,

Over many a quaint and curious volume of endstation notebook lore— while he nodded, nearly napping, suddenly there came a tapping,

As of someone gently rapping, rapping at the 2-ID-D hutch door.

"'Tis some user," he muttered, "tapping at the D hutch door— Only this and nothing more."

Presently his soul grew stronger; hesitating then no longer, "Sir," said he, "or Madam, truly your forgiveness I implore;

But the fact is I was napping, and so gently you came rapping, And so faintly you came tapping, tapping at the D hutch door,

That I scarce was sure I heard you"— here he opened wide the D hutch door;—

Darkness there and nothing more.

Deep into that darkened hutch peering, long I stood there wondering, fearing,

Doubting, dreaming dreams no staff ever dared to dream before;

But the silence was unbroken, and the stillness gave no token,

And the only word there spoken were the whispered words "Just one more (scan)?"

This I whispered, and an echo murmured back the word, "Just one more (scan)?"—

Merely this and nothing more.

Soon again he heard a tapping somewhat louder than before. "Surely," said he, "surely that is something at my D hutch door;

Open here, he punched the button, when, the door moved with a whoosh, In there stepped a stately RAVEN of the saintly days of yore;

Perched upon a bust of Roentgen just inside the D hutch door— Perched, and sat, and nothing more.

Then this ebony bird beguiling my sad fancy into smiling,

By the grave and stern decorum of the countenance it wore, "Though they crest be shorn and shaven, thou," he said, "art"

sure no craven

Ghastly grim and ancient RAVEN wandering from the PSCs Nightly shore—

Tell me what they lordly name is on the Night's Plutonian shore!

Quoth the RAVEN "Faster more!"

Much he marveled this ungainly fowl to hear discourse so plainly,

The black bird's answer had much meaning—scan a chip, and do it quickly, two fornights, that is all;

Then the bird said "Faster more!"

Startled at the stillness broken by a suggestion so aptly spoken,

"Better than 10 nm resolution," said the scientist, "Ptychographic imaging is the token, tomographic in 3D, we shall see, we shall see."

In his mind the gigabytes were flying, out of the detector quite a lot, as he sat down to design,

The Velociprobe 2.0 for the beamline. Searching the hutch to close the door, he heard the RAVEN cry

"faster more, faster more!"

The authors both thank and apologize to E.A. Poe.

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A-35
Direct LN2-cooled Double Crystal Monochromator

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A liquid-nitrogen-cooled (LN) x-ray double crystal monochromator has been designed and built for the high-power load damping wiggler ISS beamline of the NSLS2. It was designed with a direct liquid nitrogen-cooled first crystal to dissipate the maximum heat load of 2 kW, and with indirect braid liquid nitrogen cooling for the second crystal. It is designed to operate for beam energies from 5 to 36 keV with fixed exit beam mode, and for QEXAFS compatibility with channel cut mode. It is designed to rotate the Bragg axis using an AC servo motor and achieve up to 10 Hz scan.

A-36
areaDetector: What's New?

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Recent enhancements to the EPICS areaDetector module will be presented.

- New compression plugin that supports JPEG, Blosc, and Bitshuffle/LZ4 compression.
- Enhanced ImageJ pvAccess viewer that can display compressed NTNDArrays. This can dramatically reduce network bandwidth.
- Direct Chunk Write of pre-compressed NDArrays to HDF5 files, significantly improving performance.
- New ADGeniCAM base class for any GeniCAM camera. This greatly simplifies the drivers for GenICam cameras using the open-source Aravis, AVT Vimba, and FLIR Spinnaker libraries.
- Enhanced ADEiger support for the Dectris Eiger detector.

A-37
Vortex-ME7 SDD Spectrometer: Design and Performance

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The Vortex-ME7 7-element SDD spectrometer has been developed for synchrotron beam applications, which use absorption x-ray spectroscopy and micro-beam x-ray fluorescence in x-ray micro- and nano-analysis fields and which require spectrometers with high energy resolution, large solid angle and high count rate performance.

For the Vortex-ME7 we have developed new 0.5 mm thick 50 mm^2 Vortex® SDD, which has square shape and allows to minimize the SDD array dead area. Another feature of this new SDD is ultra-short signal rise. This SDD is integrated with front-end ASIC Cube preamplifier and due to very short signal rise time of the SDD and high input trans-conductance of the Cube preamplifier it provides high count rate capability and excellent energy resolution at extremely short peaking times.

High performance of the Vortex-ME7 SDD spectrometers could be fully realized in combination with new adaptive pulse processing technique, such as the FalconX (developed by XIA LLC) and the Xpress3 (developed by Quantum Detectors).

The data concerning the design and performance of the Vortex-ME7 SDD spectrometer as well as other versions of the multi-elements SDD arrays utilizing new square shape Vortex® SDD will be presented.

A-38
Sub-20-nrad Stability of LN_2-cooled Horizontal and Vertical Offset Double-crystal Monochromators

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The continuous advance towards diffraction-limited synchrotrons and free-electron-laser (FEL) sources requires beamline components with ever-increasing optical and mechanical performance. One of the key aspects for the latter is the angular vibration amplitude, which determines the positional stability of the x-ray beam at the experiment and affects its spatial coherence.

We have developed compact and mechanically rigid designs for liquid-nitrogen-cooled horizontal and vertical offset double-crystal monochromators (DCM) for the DIAD beamline at Diamond Light Source and for the ANATOMIX beamline at Synchrotron SOLEIL, respectively. For the latter one, an *in situ* differential interferometer setup directly measures the pitch and roll parallelism between the first and the second crystal under operating conditions with liquid-nitrogen flow and at vacuum pressures below 10^{-8} mbar. A similar test setup is used for in-house acceptance tests of all monochromators. Factory measurements for both monochromator types at moderate LN_2 flow rates show a stability of the relative pitch of <25 nrad RMS (0.1 to 10 kHz) and first relevant resonant frequencies well above 100 Hz. At lower flow rates, still sufficient to dissipate several hundred watts of heat load, an angular stability of about 15 nrad RMS is achieved.

A-39

Mechanical Design and Test of a Capacitive Sensor Array for 300-mm Long Elliptically Bent Hard X-ray Mirror with Laminar Flexure Bending Mechanism

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A dynamic mirror bender Z7-5004 to perform initial test for x-ray zoom optics has been designed and constructed as a part of the Argonne Laboratory Directed Research and Development (LDRD) project at the APS. Using a compact laminar overconstrained flexure bending mechanism [1,2] and a capacitive sensor array, the shape of this 300-mm-long elliptical mirror is designed to be tunable between curvatures with radii of ~0.525 and ~74 km. To ensure bender's positioning reproducibility and to monitor the mirror's surface profile, a capacitive sensor array is applied to the mirror bender [3].

In this poster, we describe the mechanical design and test setup of a capacitive sensor array for the developed precision, compact mirror bender. Finite element analyses and preliminary test results of the capacitive sensor array for the compact mirror bender are also discussed in this poster.

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A-40

Machine Learning Enabled Advanced X-ray Spectroscopy in the APS-U Era

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The Advanced Photon Source Upgrade (APS-U) will deliver x-rays that are between 100 and 1,000 times brighter than today's top synchrotron facilities, and sub-micron beamsize. This would open up scientific frontiers by enabling composition mapping, phase identification mapping, and electronic structure mapping with sub-micron spatial resolution simultaneously by using multi-modal advanced x-ray spectroscopic techniques to be developed in this proposal. The exceptional characterization techniques would dramatically accelerate materials research and discovery; however, this development would result in significant quantities of data (200 Gbit/per day). Here, we outline a roadmap to apply machine learning trained on high-fidelity simulated data to tackle the interpretation of experimental data, with a goal of achieving real-time data interpretation and experiment steering capabilities.

This research used resources 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, and the Canadian Light Source and its funding partners.

A-41

UHV Optical Chopper and Synchrotron X-ray Scanning Tunneling Microscopy Implementation

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Commissioing of XTIP, world's first dedicated beamline for synchrotron x-ray scanning tunneling microscopy (SX-STM) is underway at the Advanced Photon Source. Here we present ongoing progress of developing two crucial components for XTIP, a UHV compatible optical chopper and a low temperature scanning tunneling microscopy (STM). The optical chopper which will be positioned on x-ray beam path operates at over 3 kHz and under UHV environment. It consists of its main structural stainless steel body, optical sensor as well as chopper plate which has periodic opaque blades rotating circularly to block x-rays. The blades are coated with gold so that it will absorb soft and hard x-rays to make it opaque to x-rays. Another important part in this beamline is implementation of STM. We successfully tested the newly designed synchrotron x-ray STM by imaging HOPG and single crystal metals. Therefore, based on current progress of beamline construction, we will be able to perform the final test of the beamline and the STM working together with x-ray.

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.

Materials Science

A-42

X-ray Topography and Crystal Quality Analysis on Single Crystal Diamond Grown by Microwave Plasma Assisted Chemical Vapor Deposition

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Since decades ago, diamond has shown its value in electronics materials field. As synthesizing large size high quality single crystal diamond is facing multiple challenges, measurements through x-ray topography technique provides a best feedback to crystal growth conditions and growth qualities.

In this research, single crystal diamond is grown based on both lateral out and mosaic growth method by microwave plasma assisted chemical vapor deposition (MPACVD), measured by high resolution and small spot size (300μm) x-ray diffraction (HR μ-XRD) mapping technique at Michigan State University, and measured with x-ray topography (XRT) at 1-BM APS.

Samples are prepared mostly 400 top surfaced and perpendicular to the incident white beam x-ray. The exposure of x-ray is controlled via a fast shutter for as short as millisecond exposure. XRT pictures and XRD mapping data on both high pressure high temperature (HPHT) seeds and CVD grown diamond samples are compared to show crystal quality evolved via diamond growth. XRT films show clear (100) diamond normal surface Laue patterns, which are compared and matched with simulated diamond Laue pattern. Each XRT spot image shows detail textures that suggest how dislocations travel from the bottom surface through the top surface. XRT images are also compared to birefringence and differential interference contrast microscopy (DICM) images in details. Bundles of dislocations at variety of Burger's vectors are analyzed for multiple diamond samples, indicating the preferred orientation of traveling of dislocations from HPHT seed to CVD grown diamond. Preliminary XRT images suggest a new set up of XRT experiment that moves the film at a farther and selected specific direction towards the samples will provide much clearer XRT images, and splitting the x-ray beam will give an opportunity on imaging larger samples for smoother images. Preliminary images also suggest dislocations get less when grown from HPHT seed to CVD diamond layer, and in preferred orientations, which provides feedback on next steps diamond growth towards the goal of large size and high quality CVD diamond.

A-43

In situ X-ray Tomography of Pack Cementation for Analysis of Kirkendall Porosity Formed during Titanium Deposition on Nickel Wires

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Pack cementation is a type of chemical vapor deposition where the substrate is buried in a powder mixture containing a halide activator and the source of the material to be deposited. By depositing titanium on Ni wires and subsequently homogenizing them a hollow microtube can be created by harnessing the Kirkendall pores formed during deposition and homogenization. Some of these pores in higher wire sizes (75 and 100 μm initial diameter) form during the vapor phase deposition of titanium which makes them difficult to analyze [1–5]. To detect the mechanism by which these pores form a series of novel *in situ* experiments involving 75 μm and 100 μm pure Ni wires were conducted in which tomographic scans were collected as titanium is deposited on the substrate. Experiments on 75 μm wire were conducted for 4hrs and that for 100 μm wire were conducted for 8hrs in which radiographs of the substrate surrounded by the powder mixture were obtained. 4D visualization of the data establishes a mechanism for the formation and evolution of pores during chemical vapor deposition when the substrate is spatially symmetric and geometrically confined.

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A-44

In situ and *Operando* Bragg Coherent Diffractive Imaging at APS 34-ID-C

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Unique sensitivity to lattice of Bragg coherent diffractive imaging (BCDI) enables us to reveal inhomogeneous lattice distortion and localized defects inside materials [1]. Therefore, BCDI has been employed on various samples such as metals, metal oxides, and minerals in order to obtain three-dimensional maps. In recent years, in-situ and operando measurements became major BCDI experiments at the 34-ID-C beamline in the Advanced Photon Source (APS) to address scientific questions on physics, chemistry, and material science. In this talk, I will introduce *in situ* and *operando* capabilities and recent experimental results on *in situ* and *operando* BCDI which are performed at the APS 34-ID-C beamline [2–10]. In addition, some estimates of BCDI in the future will be discussed.

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A-45

Stress-driven Structural Dynamics in a Zr-based Metallic Glass

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Glassy materials have been shown to undergo a monotonous slowing in their structural dynamics with age [1]. This principle has been extended to metallic glasses and the existence of a universal time-waiting time-temperature superposition principle that spans compositions and temperatures has been shown [2,3]. This work shows that the application of a nominally elastic mechanical stress breaks this universal behaviour. *In situ* x-ray photon correlation spectroscopy (XPCS), conducted at the Advanced Photon Source, show the existence of instances of intermittent slow and fast dynamics, which are on an average slower than the unstressed case. We also show a direct correlation between average structural dynamics and the applied stress magnitude. Even the continued application of stress over several days does not exhaust structural dynamics. A comparison with a model Lennard-Jones glass under shear deformation replicates many of the experimental features and indicates that local and heterogeneous microplastic events are causing the strongly non-monotonous relaxation dynamics.

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A-46

Fast *in situ* 3D Characterization of Nano-materials with X-ray Full-field Nano-tomography: Latest Developments at the Advanced Photon Source

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The transmission x-ray microscope (TXM) at beamline 32-ID of the Advanced Photon Source beamline at Argonne National Laboratory has been tailored for high throughput and high spatial resolution *in operando* nano-tomography experiments [1]. Thanks to a constant

R&D effort during the last five years of operations, it emerged as a highly scientific productive instrument, especially in the domain of Materials Science and a leader in term of spatial resolution with sub 20 nm resolving power in 3D, with full dataset collection speed that can be as short as 1 min.

The TXM benefits from the in-house development of cutting-edge x-ray optics, complex opto-mechanical components and a suite of software including TomoPy, an open-sourced Python toolbox to perform tomographic data processing and image reconstruction, and others based on machine learning to push the limit of 3D nano-imaging while reducing the total x-ray dose. It operates either with a fast moderate spatial resolution (40–50 nm) mode with a large field of view of ~50 µm or with a very high spatial resolution of 16 nm and a smaller field of view of ~10 µm.

This poster presentation will give an overview of experiments covering many scientific fields like *ex* and *in situ* battery characterization [2–4], dynamic experiments with one-minute temporal resolution on cement formation, crystal growth / dissolution phenomena [5], neuroscience [6], etc.

In addition, a new projection microscope currently under development at 32-ID and expected to be operational by September 2019 will be introduced. This new instrument will provide high-speed full-field nano-tomography targeting 20 nm spatial resolution and will operate in phase contrast mode (holography). With a high coherent synchrotron source, this technique is proven very efficient for characterizing low-Z materials like Li oxide, black carbon or polymers. A comparison of such materials characterization with TXM and Projection Microscopy will be shown.

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A-47

Measuring Relative Crystallographic Misorientations in Mosaic Diamond Plates Based on White Beam X-ray Diffraction Laue Patterns

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The electrical and thermal properties of diamond make it a promising material for new generation electronic devices. Accelerated progress in this field requires significant improvement on the development of large area single crystal diamond substrates. This work explores the mosaic technique, where single crystal substrates are grown by microwave plasma assisted chemical vapor deposition over an assembly of individually tiled substrates. Initial crystallographic alignment is critical in this process, as well as establishing the conditions where the relative misorientation between the plates is reduced as the sample thickness is increased. The analysis presented in this study measures the relative misorientations by interpreting the diffracted Laue patterns over a series of plates corresponding to cumulatively grown layers over a mosaic substrate. The monochromatic x-ray source was supplied by beamline 1-BM-B at the APS. Pattern analysis was performed using LauePt [1] software, where pattern matching can be obtained by approximating the sample rotation relative to the incident beam. The adjustments required to align the geometric center of each crystallographic tile at the observed diffraction spots directly correspond to the relative misorientation in the mosaic plates. Results directly confirm initial misorientations in the order of 0.6 ± 0.3 degrees, and a reduction in misorientation as the sample thickness is increased over time. Preliminary results show an effective elimination of the initial relative misalignment along at least one of the three possible misorientation axis. The straightforward process demonstrates the feasibility of the measuring technique as an effective approximation, and as a two dimensional visualization extension over the standard x-ray rocking curve techniques for determining the large scale misorientation in mosaic substrates. We expect these results to lead toward successful fabrication of large area single crystal diamond wafers.

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A-48

Understanding the Dynamics of Mabs and Excipients at the Air-water Interface

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The adsorption of therapeutic monoclonal antibodies (mAbs) at the air-water interface is central to the production and use of antibody-based pharmaceuticals. Air-water interfaces are generated during the production, processing and storage of therapeutic formulations by pressure driven shear stress or shaking [1,2]. When an air-water interface is created, the antibodies will expose their hydrophobic residues to the gas phase leading to partial unfolding, interfacial aggregation, irreversible adsorption and recruitment of additional proteins from the solution phase [3]. This leads to decreased yields in production as well as a shortened shelf life of these therapeutic drugs. Furthermore, the adsorption phenomenon will result in the conformational degradation of the antibody, where the loss of secondary and tertiary structure can result in diminished activity and promote immunogenicity, inhibiting the efficacy of the biologic drugs. In order to solve this problem and enhance the physical stability of therapeutic monoclonal antibodies, the pharmaceutical industry uses a multicomponent formulation that includes surface active excipients [4].

The aim of this work [5] was to explore the competitive adsorption process between surfactant and two monoclonal antibody (mAb) proteins, mAb-1 and mAb-2. Pendant bubble tensiometer was used to characterize the equilibrium and dynamic surface tension. Additionally, a double-capillary setup of the pendant drop tensiometer was used to exchange mAb solutions with histidine buffer. X-ray reflectivity (XR) was used to measure adsorbed amounts and understand the molecular configurations of the adsorbed molecules. A box-refinement method based on the model independent approach was used to predict the structural information on an angstrom scale. In addition, XR was used for the first time to reveal the orientation of the mAb molecules at the air-water interface. The mAbs adsorbed in their “flat-on” orientation at early time scales and reoriented to “side-on” for higher mAb concentration.

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A-49

Carbon-coated High Capacity Li-rich Layered $Li[Li_{0.2}Ni_{0.2}Mn_{0.5}Fe_{0.1}]O_2$ Cathode for LIBs

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Rechargeable lithium ion batteries (LIBs), currently used both in electronic devices and in hybrid/electric vehicles (HEV/EV) are made up of expensive and toxic cathode materials such as layered lithium cobalt oxide ($LiCoO_2$) and $Li[Li_{0.2}Ni_xMn_yCo_z]O_2$ (NMC), mostly because of the presence of Ni and Co elements [1,2]. Among other cathode materials, polyanion compounds ($LiFePO_4$, $LiVO_3$, Li_2FeSiO_4, etc.), which are suffering from lower theoretical capacity for battery applications requiring high energy and power densities, have also been studied as a promising LIB cathode candidates due to their safety, good stability and low cost, compared to commercial $LiCoO_2$ and NMC [3]. In this aspect, $Li[Li_{0.2}Ni_xMn_yFe_z]O_2$ (NMF) Li-rich layered oxide cathode has been attracting intensive attention due to its high capacities of ~250 mAh/g with lower cost and better safety [4]. However, its low rate capability resulting from its low electronic conductivity caused by the insulating $Li[Li_{1/3}Mn_{2/3}]O_2$ component [5] and the thick solid-electrolyte interfacial (SEI) layer formed when the cell is operating at 4.8V [6] constitute an impediment in commercializing these cathodes for EV and HEV industries. One approach to overcome the SEI layer thickness and improve the surface conductivity is well known to coat the cathode surface with conductive agents [3].

We present the electrochemical performance of the lithium-rich layered $Li[Li_{0.2}Ni_{0.2}Mn_{0.5}Fe_{0.1}]O_2$ (NMF251) cathodes coated with different carbon sources as conductive agents, such as citric acid (CA), graphene oxide

(GO), and 50%CA&50%GO in this study. Also, structural, morphological and phase analysis of the materials correlated to the cell performance will be discussed with the results from x-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive x-ray analysis (EDX), thermogravimentric analysis (TGA), in addition to their electrochemical characterizations such as galvanostatic charge/discharge measurements, cyclic voltammetry (CV), and impedance spectroscopy (EIS).

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A-50

The Mechanism of Eutectic Modification by Trace Impurities

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In the quest toward rational design of materials, establishing direct links between the attributes of microscopic building blocks and the macroscopic performance limits of the bulk structures they comprise is essential. Building blocks of concern to the field of crystallization are the impurities, foreign ingredients that are either deliberately added to or naturally present in the growth medium. While the role of impurities has been studied extensively in various materials systems, the inherent complexity of eutectic crystallization in the presence of trace, often metallic impurities (eutectic modification) remains poorly understood. In particular, the origins behind the drastic microstructural changes observed upon modification are elusive. Herein, we employ an integrated imaging approach to shed light on the influence of trace metal impurities during the growth of an irregular (faceted–non-faceted) eutectic. Our dynamic and 3D synchrotron-based x-ray imaging results reveal the markedly different microstructural and, for the first time, topological properties of the eutectic constituents that arise upon modification, not fully predicted by the existing theories. Together with *ex situ* crystallographic characterization of the fully-solidified specimen, our multi-modal study provides a unified picture of eutectic modification. The impurities selectively alter the stacking sequence of the faceted phase, thereby inhibiting its steady-state growth. Consequently, the non-faceted phase advances deeper into the melt, eventually engulfing the faceted phase in its wake. We present a quantitative topological framework to rationalize these experimental observations.

A-51

Single Molecule Magnetic Behavior of Near Liner N,N Bidentate Dy Complex

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Atoms which have populated f type orbitals are of interest due to the under explored nature of their chemical bonding interactions and their unique magnetic and electronic properties [1]. Among these, dysprosium containing molecules have illustrated intriguing single molecule magnetic (SMM) behavior with some compounds having SMM activity blocking temperatures in excess of 80 K [2,3]. These breakthroughs, along with other recent works, has suggested that linear geometry about the Dy, which establishes a axially coordinated dysprosium complexe, enhance anisotropic behavior and SMM activity of such complexes [4]. Here we report the synthesis of a N-tethered dysprosium (III) complex, $L^{Ar}Dy(Cl)_2K(DME)_3$ ($L^{Ar} = C_6H_4[(2,6\text{-}^{i}PrC_6H_3)NC_6H_4]_2\}^{2-}$), which features a terphenyl bisanilide ligand with near linearly coordinated nitrogen atoms (N1–Dy1–N2 = 159.9°). Solid state structure, SQUID magnetic data and theoretical computational data are presented which illiterate the SMM behavior of our complex, including obtained U_{eff} values (1334 K/927 cm^{-1} and 1366 K/949 cm^{-1}) and probable relaxation pathways for our complex.

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A-52

Non-destructive 3D Grain Mapping by Laboratory X-ray Diffraction Contrast Tomography

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Determining crystallographic microstructure of a given material in 2D can be challenging. Further extending such an investigation to 3D on meaningful volumes (and without sample sectioning) can be even more so. Yet reaching this insight holds tremendous value for 3D materials science since the properties and performance of materials are intricately linked to microstructural morphology including crystal orientation. Achieving direct visualization of 3D crystallographic structure is possible by diffraction contrast tomography (DCT), which was for a long time only available at a limited number of synchrotron x-ray facilities around the world.

Laboratory diffraction contrast tomography (LabDCT) technique with a Zeiss Xradia Versa x-ray microscope opens up a whole new range of possibilities for studies of the effect of 3D crystallography on materials performance in the laboratory. Using a polychromatic x-ray source, LabDCT takes advantage of the Laue focusing effect, improving diffraction signal detection and allows handling of many and closely spaced reflections. Grain morphology, orientation and boundaries of metals, alloys or ceramics can be characterized fully in 3D.

LabDCT opens the way for routine, non-destructive and time-evolution studies of grain structure to complement electron backscatter diffraction (EBSD). Crystallographic imaging is performed routinely by EBSD for metallurgy, functional ceramics, semi-conductors, geology, etc. However, in most cases it is difficult for EBSD to investigate microstructure evolution when subject to either mechanical, thermal or other environmental conditions.

The non-destructive nature of LabDCT enables the observation and characterization of microstructural response to stimuli (stress, thermal, radiation) of one and the same sample over time. Combination of LabDCT with conventional absorption contrast imaging enables a wide range of microstructural features to be characterized simultaneously and provides complementary information about the observed microstructure. Aside from introducing the fundamentals of the technique and its implementation on a laboratory scale, we will present a selection of LabDCT applications with particular emphasis on how its non-destructive operation can facilitate a better understanding of the relation between structure and property for polycrystalline materials.

A-53

Investigating Atomic Structures of Mesoscale and Highly Curved Two-dimensional Crystals by Surface X-ray Nanodiffraction

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Ever since the storming rise of graphene, the expanding list of two dimensional material family as predicted by theorists has been experimentally verified almost in every few months in the last years. Most fundamental properties of 2D atomic thin crystals, such as morphology/geometric profiles, electronic/magnetic transports and optoelectronic responses can be investigated by various optically excited and surface force sensitive techniques like Raman/IR spectroscopy and AFM/STM probes. However, determining atomic structures of versatile 2D crystal surfaces and interfaces in the burgeoning 2D heterostructure materials remains very challenging. So far, high-resolution cross-section TEM is still the most popular and viable method to map out surface/interface atomic structures of 2D crystal and other derivative materials although the delicate interface bonding can be undesirably vulnerable to electron-beam effects. Synchrotron-based surface x-ray diffraction, in particular crystal truncation rod (CTR) technique, can render a complete and precise atomic structure of single crystals and high quality epitaxial thin films/heterostructures in non-destructive manner. Nevertheless, the miniature lateral dimension (e.g., less than a few to tens of microns) of most 2D flakes and heterostructures makes conventional surface x-ray diffraction almost impractical to map out the complete Bragg rod so as to extract the complete atomic structures. Moreover, structural and electronic phases of some unique 2D crystals are strikingly controllable by strain applied by the underlying substrate or support when it has a large surface curvature, which for certain throws another big technical barrier for any surface-sensitive x-ray techniques.

High-brilliance, high flux synchrotron source and state-of-art focusing optics capable of routinely realizing nanobeam below 100 nm makes x-ray nanodiffraction, even surface x-ray nanodiffraction become practical and user-accessible. In this talk, I will discuss the feasibility

of surface x-ray nanodiffraction measurements, and then demonstrate two most recent intriguing practices on investigating 2D atomic thin crystal and Lego-style 2D heterstructures. In one case, surface nanodiffraction helps to map out the complete specular CTR of a high quality graphene-hexagon BN heterostructure. The resolved interfacial atomic structures suggest a subtle variation of interfacial van-der-waals bonding between exfoliated and CVD grown 2D thin crystals. In another example, surface nanodiffraction allowed for precise determining in-plane lattice expansion of miniature MoS2 2D flakes vapor grown on highly curved glass spheres, which provides an excitingly new approach to effectively manipulate electronic band valley structures [1]. In summary, surface x-ray nanodiffraction brings about significant opportunities for us to explore new two-dimensional materials, unravel emergent phenomena, and develop novel functionalities.

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Nanoscience and Nanotechnology

A-54

Photoinduced, Transient Disordering in CdSe Nanostructures Characterized via Time-resolved X-ray Diffraction (TR-XRD)

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One of the most fundamental changes imparted upon materials in the nanoscale form is a reduction in thermodynamic stability, owing to a dramatic increase in surface-to-volume ratio. This reduced stability has practical implications in the operation of commercial display and lighting applications that utilize nanocrystals (NCs) and operate at high carrier injections. Previously, we have used transient x-ray diffraction (TR-XRD) conducted at APS beamline 11-ID-D to show that photoexcitation at elevated fluences can induce transient disordering, or melting, of NCs [1]. Since melting of the NC lattice can affect NC electronic structure, photophysics, and dynamics, it is critical to understand fluences that produce disordering, as well as the impacts of NC size, shape, and composition.

Recently, two-dimensional colloidal semiconductor NCs known as nanoplatelets (NPLs) have emerged as a promising advancement over spherical NCs in optoelectronic applications. NPLs feature extremely narrow photoluminescence linewidths that are only slightly inhomogeneously broadened, as NPL ensembles with little to no thickness dispersion are produced. Meanwhile, NPLs retain many of the advantageous properties of spherical NCs, such as solution processability and size-tunable bandgaps. However, it is not clear how anisotropic structure affects thermodynamic stability, especially considering the presence of high surface-energy corners and edges relative to larger, flat surfaces. Using TR-XRD, we probe the thermal response to photoexcitation in NPLs and find that transient disordering occurs anisotropically in NPLs. Notably, the (100) plane experiences very little disordering, suggesting that the NPL thickness (defined by the [100] direction) is unperturbed by photoexcitation, whereas lattice directions with a perpendicular component show transient disorder. These transient findings are in contrast to temperature-dependent static XRD measurements conducted at APS Sector 5, which show that NPLs melt isotropically under equilibrium thermal heating conditions.

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A-55

GI-S/WAXS Study of the Effects of Silica Nanopore Confinement and Tethering on Crystallization and Transport Behavior of 1-butyl-3-methylimidazolium [BMIM]-based Ionic Liquids

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Ionic liquids (ILs) are molten organic salts of widespread interest for separations, energy storage materials and catalysis due to their extremely low volatility, good thermal stability and tunable solvent properties. However, utilizing bulk ILs presents practical challenges due to their unknown toxicity, high cost, and difficult solute recovery. Therefore, supported ILs in nanoporous supports are being developed to overcome many disadvantages and promote

their potential for separation and catalysis. The present work gives insights of how silica mesopore confinement affects the crystallization behavior of the two selected 1-butyl-3-methylimidazolium [BMIM]-based ILs by using in situ GIWAXS experiment performed at the Advanced Photon Source (APS).

Confinement of ILs was investigated using mesoporous silica thin films prepared by templating with Pluronic surfactant P123. Vertically oriented, accessible pores (8–9 nm in diameter) were achieved by synthesizing the thin films on a neutral chemically modified surface of crosslinked layer of P123. Titania-doped silica thin films with vertical pores about 3 nm in diameter are obtained with a similar principle but using cationic surfactant cetyltrimethylammonium bromide (CTAB) and different approaches to pore orientation. The development of the porous structures of the films were studied with *in situ* GISAXS at APS. Some of the porous film was modified by covalently tethering 1-(3-trimethoxysilylpropyl)3-methylimidazolium chloride to the pore wall. The crystallization of [BMIM] ILs with Cl^- and PF_6^- counterions, confined in both modified and unmodified P123 films, were studied by *in situ* GIWAXS at APS. Both polymorphism and crystal transition temperatures were changed by confinement for both ILs. The interactions between ILs and the silica surface, and molecular rearrangement due to nanoconfinement, are believed to be the main reasons for the observed changes. This has important implications for using ILs as ion conductors and catalyst supports, and selecting process temperatures. As an illustration of this, an electrochemical impedance spectroscopy (EIS) study shows that confined [BMIM][PF_6] exhibits selective surface resistance towards hydrophobic and hydrophilic redox probes. Transport selectivity is strongly affected by tethering of ILs to the pore walls. This suggests that confinement of [BMIM][PF_6], especially when covalently tethered, can be used to enhances their selectivity towards transport of solutes in separations, sensing and battery applications.

A-56
Convolutional Neural Network Based Super Resolution for X-ray Imaging

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The transmission x-ray microscope (TXM) at the Advanced Photon Source (sector 32-ID) in the Argonne National Laboratory has been upgraded to achieve a spatial resolution of sub 20 nm. However, x-ray acquisition at the TXM's maximum capacity still remain a challenging task. In particular, reconstructions deduced from the TXM's maximum limit show various forms of inconsistencies ranging from motion/drift artifacts to beam damage. Accordingly, in this contribution, we propose the use of convolutional neural network (CNN) based super resolution to enhance the features of low resolution x-ray images. Our overarching goal will be to use the CNN approach to learn the mapping from the low-resolution (LR) to the high-resolution (HR) from few hundreds of artifacts free HR x-ray images. Then in the subsequent beam runs only the LR images will be acquired and the network mapping will be employed to scale-up these LR images. Finally, the efficacy of our CNN based super resolution technique will be evaluated with the aid of quantitative metrics such as the fourier ring correlation (FRC), the peak signal-to-noise ratio (PSNR), and the structural similarity (SSIM) index.

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Technique

A-57
A Dedicated ASAXS Facility at NSF's ChemMatCARS

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In this poster, I will present recent developments at NSF's ChemMatCARS (Sector 15, APS) in bringing up a dedicated anomalous small angle x-ray scattering (ASAXS) facility for researchers. The developments include addition of new hardware to existing SAXS equipment and the development of complete software suite (**XAnoS: X**ray **A**nomalous **S**cattering) for ASAXS data collection and analysis. The software suite is developed in Python and can be freely available upon request here: https://chemmatcars.uchicago.edu/page/software.

The first two years of the development is seed funded through the Institute of Molecular Engineering at the University of Chicago. I will also present some of the recent exciting studies done at the facility on studying ion-distributions in polyelectrolytes.

NSF's ChemMatCARS Sector 15 is supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1834750. 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, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

A-58
Liquid Surface/Interface Scattering Program at NSF's ChemMatCARS

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A liquid surface/interface scattering instrument has been operational since 2002 at NSF's ChemMatCARS Sector 15-ID of the Advanced Photon Source (Argonne National Laboratory). The instrument can perform all the principal x-ray techniques to study liquid-vapor and liquid-liquid interfaces. It has been used to investigate a wide range of chemical and materials interfacial phenomena, including those relevant to the environment, biomolecular materials, life processes, self-assembly, and directed assembly for tailored functionality.

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A-59
Python Software Development at GSECARS

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One of the bottlenecks of efficient usage of beamtime at high-brilliance synchrotron sources is software. This includes software for beamline control and data collection, for preliminary on-the-fly data analysis, for collection of meta-data, and for solving problems which may arise. This is specifically an important issue for users of the GSECARS diamond anvil program, who perform x-ray diffraction measurements at high-pressure and high-temperature conditions. These studies require simultaneously controlling and monitoring multiple parameters related to the sample position, pressure, temperature, and often synchronizing the diffraction measurements with spectroscopic, electric or other measurements. For this reason, we have been developing new user-friendly GUI based software, simplifying the data collection and treatment every step of the way throughout the experiment and after. The software is developed in Python so that the code is open source and can be used and/or modified by others with no required purchase of software.

We have further developed our automatic logging capabilities, allowing users to monitor unlimited EPICS events and register any experimental information in a convenient interactive format. Thus, the users can go back and find all the relevant meta-data collected along with the diffraction, spectroscopic and optical imaging data. This is especially useful in cases where quick successive measurements are taken, or multiple detectors are used at the same time, and the users cannot write down all the information within such a short time span, allowing them to focus on making split-second decisions. We have also improved the 2D mapping visualization of diffraction data within DIOPTAS [1]. Users can now easily overlay up to three different ROIs (or mathematical combinations of ROIs) with an optical image, comparing multiple diffraction patterns collected at different locations within the sample chamber. We have developed software for performing pulsed laser-heating, heating to 1000s of Kelvins while at high-pressure with significantly reduced risk to the diamond anvils. Before this software was developed, the process required two experienced users to operate, but now a single user, trained on the spot, can operate it alone.

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A-60
On the Use of Automatic Differentiation for Phase Retrieval

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The recent rapid development in coherent diffraction imaging (CDI) methods has enabled nanometer-resolution imaging in a variety of experimental modalities. Image reconstruction with such CDI methods involves solving the phase retrieval problem, where we attempt to reconstruct an object from only the amplitude of its Fourier transform. This can be framed as a nonlinear optimization problem which we can solve using a gradient-based minimization method. Typically, such approaches use closed-form gradient expressions. For complex imaging schemes, deriving this gradient can be difficult and laborious. This

restricts our ability to rapidly prototype experimental and algorithmic frameworks.

In this work, we use the *reverse-mode automatic differentiation* method to implement a generic gradient-based phase retrieval framework. With this approach, we only need to specify the physics-based forward propagation model for a specific CDI experiment; the gradients are exactly calculated automatically through a sequential application of the chain rule in a *reverse pass* through the forward model. Our gradient calculation approach is versatile and can be straightforwardly implemented through various deep learning software libraries (TensorFlow, Pytorch, Autograd, etc.), allowing for its use within state-of-the-art accelerated gradient descent algorithms. We demonstrate the generic nature of this phase retrieval method through numerical experiments in the transmission (far-field and near-field), Bragg, and tomographic CDI geometries.

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A-61

Strain Mapping in Single Crystals from Maps of Rocking Curves at Beamline 1-BM of the Advanced Photon Source

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Shifts in rocking curves can be mapped at beamline 1-BM. From shifts obtained at two azimuthal sample rotations , but from the same lattice planes, one can measure both the change in Bragg spacing, Δd/d, and a lattice tilt. Any one rocking curve can be shifted due to both contributions, and from rocking curves for two azimuthal rotations one can separate the two. Typically the two azimuthal rotations are 180 deg apart. Measurements made at 90 and 270 deg can be used to confirm Δd/d. The technique was introduced by Bonse [1], and has been applied to Si [2], synthetic quartz [3,4], GaAs [5], synthetic diamond [6–8] and recently to 4H-SiC [9]. Early measurements were made with laboratory sources and film. The advent of area detectors, conditioning upstream optics and a high angular resolution goniometer at 1-BM has brought the technique into the modern era, with benefits for both resolution and speed of data taking. The set-up at 1-BM will be highlighted together with illustrative results.

A-62

Synchrotron Powder Diffraction Simplified: The High-resolution Diffractometer 11-BM at the Advanced Photon Source

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Synchrotrons have revolutionized powder diffraction. They enable the rapid collection of high quality powder diffraction patterns with tremendous resolution and superb signal to noise. In addition, the high penetration and exceptional data sensitivity possible at high-energy light sources, like the Advanced Photon Source (APS), allow exploration of trace containment levels, in-situ sample environments and crystallographic site occupancies which previously demanded neutron sources. Despite all these advantages, relatively few scientists today consider using a synchrotron for their powder diffraction studies. To address this, the high resolution synchrotron powder diffractometer beamline 11-BM at the APS offers rapid and easy mail-in access for routine structural analyses with truly world-class quality data [1]. This instrument offers world-class resolution and sensitivity and is a free service for non-proprietary users [2]. The instrument can collect a superb pattern suitable for Rietveld analysis in less than an hour, is equipped with a robotic arm for automated sample changes, and features variable temperature sample environments. Users of the mail-in program typically receive their high-resolution data within two weeks of sample receipt. The diffractometer is also available for on-site experiments requiring more specialized measurements.

This presentation will describe this instrument, highlight its capabilities, explain the types of measurements currently available, as well as recent significant improvements to the instrument's performance. We will discuss plans to improve access and the available sample environments and collection protocols. We are particularly interested in seeking input from potential users within the powder diffraction community.

More information about the 11-BM diffractometer and its associated mail-in program can be found at our website: https://11bm.xray.aps.anl.gov.

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CNM POSTER ABSTRACTS

Chemistry

C-1

Photoregeneration of Biomimetic Nicotinamide Adenine Dinucleotide Analogues via a Dye-sensitized Approach

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The two-step photochemical reduction of an acridinium-based cation ($2O^+$) to the corresponding anion ($2O^-$) was investigated by utilizing the dye-sensitized approach which involving attachment of dye-catalysts ($2O^+$-COOH) to the surface of a p-type wide band semiconductor (p-NiO). The cation ($2O^+$) and corresponding radical ($2O^-$) were synthesized and characterized. The results from steady-state spectroscopy revealed that the photoinduced hole injection from $2O^+$ and $2O^-$ to valance band (VB) of the NiO thermodynamically favorable. Subsequent femtosecond spectroscopy was utilized to investigate the kinetics of photoinduced hole injection from $2O^+$-COOH/NiO and $2O^-$-COOH/NiO to VB of the NiO and results showed that upon the excitation of $2O^+$-COOH/NiO at 620 nm, fast hole injection occurred within (2.8 ps) from $2O^+$-COOH/NiO into the VB of NiO Subsequently, 90% of charge separated population recombined within ~40 ps while ~10% of the charged separated population could be utilized to drive the photoinduced second electron reduction. In the case of the second electron reduction, $2O^-$-COOH/NiO predominantly absorbed in the UV range (310 nm) and upon the excitation of $2O^-$-COOH/NiO the electron transfer from the conduction band of NiO to the radical could be observed due to the simultaneous excitation of the NiO. The results of this work indicate that the two-step photochemical reduction of $2O^+$ to the corresponding hydride form (2OH) can be achievable, opening the possibility of using such a dye-sensitized approach for regeneration of nicotinamide adenine dinucleotide analogues in enzymatic and chemical catalysis.

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Condensed Matter Physics

C-2

Spintronic Terahertz Emission by Ultrafast Spin-charge Current Conversion in Organic-inorganic Hybrid Perovskites/ Ferromagnet Heterostructures

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Terahertz (THz) technologies hold great promise to the development of future computing and communication systems. The ideal energy-efficient and miniaturized future THz devices will consist of light-weight, low-cost, and robust components with synergistic capabilities. Yet it has been challenging to realize the control and modulation of THz signals to allow system-level applications. Two-dimensional organic-inorganic hybrid perovskites (2D-OIHPs) have been shown to allow for facile and economical, solution-based synthesis while still successfully maintaining high photocurrent conversion efficiency, excellent carrier mobility, low-cost chemical flexibility, pronounced Rashba-splitting, and remarkable defect tolerance. These make them promising candidates for high-performance spintronic THz devices.

Here we demonstrate the generation of THz signal waveforms from a 2D-OIHP/$Ni_{80}Fe_{20}$ heterostructure using an ultrafast laser excitation below the bandgap of 2D-OIHPs. A 180° phase shift of THz emission is observed when the polarity of the external magnetic field is reversed. In contrast to the metallic spintronic THz heterostructures, we found the asymmetry in the intensity between the forward and backward propagating THz emissions as a function of the polarity of the applied magnetic field, indicating an active control of a *unidirectional* THz emission via OIHP interface. Our study demonstrates the spintronic THz emitters using hybrid 2D-materials with synergistic functionalities, highly sensitive response function and optimized energy output, generating a paradigm shift in THz applications using solution-processed hybrid quantum materials.

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Instrumentation

C-3

Hard X-ray Transition Edge Sensors at the Advanced Photon Source

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At the Advanced Photon Source (APS), we are developing new detector arrays based on superconducting transition edge sensors (TESs) for hard x-ray energies (2 to 20 keV). TESs provide an order-of-magnitude improvement in energy resolution compared to the best semiconductor-based energy-dispersive spectrometers, while still allowing for a high count rate and spatial resolution unlike wavelength-dispersive spectrometers. These devices will enable new science, particularly in x-ray fluorescence and x-ray emission spectroscopy. We discuss the design of our prototype devices—successfully fabricated at the Center for Nanoscale Materials (CNM)—and readout system, and present our first characterization results, including quantitative comparisons with the silicon-drift detectors currently available at the beamline to APS users.

This research is funded by Argonne National Laboratory LDRD proposal 2018-002-N0: Development of a Hard X-ray Spectrometer Based on Transition Edge Sensors for Advanced Spectroscopy. This research was supported by the Accelerator and Detector R&D program in Basic Energy Sciences' Scientific User Facilities (SUF) Division at the Department of Energy. This research used resources of the Advanced Photon Source and Center for Nanoscale Materials, U.S. Department of Energy Office of Science User Facilities operated for the DOE Office of Science by the Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

This work made use of the Pritzker Nanofabrication Facility of the Institute for Molecular Engineering at the University of Chicago, which receives support from Soft and Hybrid Nanotechnology Experimental (SHyNE) Resource (NSF ECCS-1542205), a node of the National Science Foundation's National Nanotechnology Coordinated Infrastructure.

C-4

A Two-dimensional Resistor Network Model for Transition-edge Sensors with Normal Metal Features

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The transition-edge sensor is a type of superconductive detector characterized by high energy resolution, owing to the sensitive resistance-temperature dependence in the superconducting-to-normal transition edge. In order to minimize the thermal noise, TESs are usually made of superconductive or bilayer materials with sub-Kelvin critical temperature. Nonetheless, some excess noise can be present. To minimize this and to tune the transition resistance slope, normal metal banks and bars are often implemented on TES films. Until now, there have been theoretical models explaining the TES transition shape by treating the device one-dimensionally or as a single body. In spite of their good agreement with experimental results, there have not been quantitative discussions on the influence of the two-dimensional (2D) features of TESs. In this work, we treat the TES as a 2D network of resistors, whose values are defined by a superconductivity two-fluid model, and study how the normal metal features influence its transition shape. We will show that the normal metal banks force the current to meander around the normal metal bars when the TES is biased low in the transition, and that at high biases the current distributes uniformly across the film. This current pattern is directly linked to the TES transition slope.

This work was supported by the Accelerator and Detector R&D program in Basic Energy Sciences' Scientific User Facilities Division at the U.S. Department of Energy and the Laboratory Directed Research and Development (LDRD) program at Argonne National Laboratory. This research used resources of the Advanced Photon Source and Center for Nanoscale Materials, U.S. Department of Energy Office of Science User Facilities operated for the DOE Office of Science by the Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

C-5

Superconducting Thin Films for Ultra-low Temperature Transition Edge Sensors

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Sensitive superconducting transition edge sensor (TES) based bolometers and calorimeters have a wide range of applications, such as cosmic microwave background observation, direct dark matter detection, and neutrinoless double beta decay search, thanks to their high energy and timing resolutions. One of the major challenges to make these detectors is the realization of superconducting films with low and controllable transition temperature (Tc). Tunable transition temperatures can be obtained by coupling bilayers or multilayers with proximity effect, doping elemental superconductors with magnetic centers, or the combination of the two. Here we will describe the results for two systems of low Tc superconducting films: the Iridium/Platinum (Ir/Pt) and Iridium/Gold (Ir/Au) bilayer or multilayer films with a target Tc ~30 mK, and Aluminum doped with Manganese (Al-Mn) or Cobalt (Al-Co) with a target Tc ~150 mK. We will present the measured superconducting transition temperatures and characteristics of these films and their dependence on the material thickness, doping level, and fabrication techniques. These results will assist future detector developments.

Work at Argonne, including use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Offices of Basic Energy Sciences, Nuclear Physics, and High Energy Physics, under Contract No. DE-AC02-06CH11357.

Materials Science

C-6

Ion Irradiation Damage in Commercially Pure Titanium and Ti-6Al-4V: Characterization of the Microstructure and Mechanical Properties

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Due to their low activation, corrosion resistance, good mechanical properties, and their commercial availability, Ti-alloys, especially the α+β alloy Ti-6Al-4V (wt%) alloy, are considered for different applications in the nuclear industry. Ti-6Al-4V is also being considered as a structural material for the beam dump for the Facility for Rare Isotope Beams (FRIB) at Michigan State University: a new generation accelerator with high power heavy ion beams. In this study, samples of commercially pure (CP) Ti and Ti-6Al-4V were irradiated at Notre Dame University using 4 MeV Ar ion beam at 25°C and 350°C. The samples irradiated at RT were exposed to two different dose rates: 0.8 dpa/h and 13.4 dpa/h and had reached the same final dose of 7.3 dpa within 1 µm of the surface. The Ti-6Al-4V samples were processed through two different thermomechanical processes: powder metallurgy (PM) rolled and additive manufacturing (AM). The latter consisted of direct metal laser sintering (DMLS) followed by hot isostatic pressing (HIP). The samples exhibited two distinctly different microstructures. The powder metallurgy (PM) rolled sample exhibited equiaxed α-phase grains with the β-phase typically present at the grain boundary whereas the additively-manufactured sample exhibited a lamellar α+β microstructure. Nano indentation measurements were carried out on the surface of the bulk samples. CP-Ti exhibited the highest irradiation induced hardening, whereas the Nano hardness of the additively manufactured Ti-6Al-4V was the most sensitive to the dose rate.

To better understand the defect structure in the irradiated samples, 3 mm thin foils were prepared for Transmission Electron Microscopy (TEM). The TEM characterization, which was performed at CNM and ORNL, showed that the <c>-component loops were only observed in the samples irradiated at high temperature. The density of the <a> loops was too high and the loops too enmeshed for quantitative characterization. *In situ* TEM irradiation at the IVEM facility was performed to further investigate the dose and temperature dependence of ion irradiation damage. CP-Ti and additively manufactured Ti-6Al-4V TEM foils were irradiated using 1 MeV Kr ions at 25°C, 360°C, and 430°C. The analysis of the results is ongoing.

C-7
Electrochemical Reduction of CO_2 on Transition Metal/P-block Compositions

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Among all the pollutants in the atmosphere, CO_2 has the highest impact on global warming and with the rising levels of this pollutant, studies on developing various technologies to convert CO_2 into carbon neutral fuels and chemicals have become more valuable. Electrochemical reduction is one of the solutions to convert CO_2 to value added hydrocarbon fuels using non-precious, earth-abundant nanocatalysts making this process cost-effective. To understand the activity of catalysts for a particular reaction, we should be able to tailor the catalyst atom by atom. With the advances in computing power and quantum modelling tools, researchers are able to design and study different types of "*in silico*" materials. Previous experimental results indicate transition metal-p block catalysts such as oxides show improved catalyst activity and desired product selectivity. However, the design principle and reaction mechanism are poorly explored.

In this work, we present a detailed computational study of electrochemical reduction of CO_2 (CO_2RR) to methane and methanol over different transition metal-p block catalysts using Density Functional Theory calculations. In addition to the catalyst structure, we studied reaction mechanisms using free energy diagrams that explain the product selectivity with respect to the competing hydrogen evolution reaction. From these diagrams, we hypothesized that transition metal oxides and sulfides favor methanol over methane formation at lower overpotentials. Furthermore, we developed scaling relations to find the key intermediate species for CO_2RR on transition metal-p block catalyst materials. We have found CO* as the descriptor (key species) from these relations and modifying the binding free energy of this species would modify the catalyst activity. We developed thermodynamic volcano plots for each product relating descriptor (CO*) binding energy to all other intermediate species binding energy to characterize and rank the activity of catalysts studied so far and determine the optimal binding energy region of the descriptor. This plot will provide guidance to our future work on improving the activity of current transition metal-p block family of catalysts and develop new catalysts for this important reaction.

We acknowledge financial and research support from the Department of Chemical Engineering at Villanova University. We are also thankful for the computational support (use of HPC/carbon cluster) from the Center for Nanoscale Materials, supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC-02-06CH1137.

C-8
Fabrication, *in situ* Biasing, Electron Holography and Elemental Analysis of Patterned and Unpatterned TiO_2 Thin Films

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TiO_2 is a metal oxide that can undergo resistive switching, a reversible change between high and low resistance states by application of a voltage bias. This behavior has promising applications in neuromorphic computing and nonvolatile memory. In order to gain a deeper understanding of the mechanism behind reversible switching and electric breakdown in TiO_2 we have fabricated samples for *in situ* biasing and Transmission Electron Microscopy, (TEM). Additionally, we have patterned thin films of TiO_2 on the nanoscale as a means to gain additional insights into the reversible breakdown through *in situ* biasing.

I will present details of the fabrication process we developed at the Center for Nanoscale Materials, (CNM). This includes both the process to pattern TiO_2 thin films and the preparation of thin films for *in situ* biasing in TEM. In order to pattern TiO_2 , we perform sequential infiltration synthesis of Al_2O_3 into block copolymers to make a patterned film of Al_2O_3 on top of thin films of TiO_2. Using reactive ion etching we transfer the Al_2O_3 pattern into the TiO_2 thin film. To prepare these patterned and unpatterned samples for *in situ* biasing we use electron beam lithography to write electrodes on top of the TiO_2 thin films. Finally, we use wet etching to back etch SiN windows

into our substrate. Additionally, I will present results from *in situ* biasing experiments. Using electron holography and electron energy loss spectroscopy (EELS) in the CNM, we have observed irreversible changes in our thin films during our biasing experiments. I will compare these results in the patterned and unpatterned TiO_2 films.

This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Science, Materials Sciences and Engineering Division. Use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

C-9

Characterization of Boron/Iron-oxide Core/Shell Structure for Boron Neutron Capture Therapy by STEM/EELS-XEDS and Mössbauer Spectroscopy

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This project is the characterization of boron/iron-oxide core/shell structured nanoparticles, for application in boron neutron capture therapy (BNCT). BNCT is a cancer treatment method using boron's ability to absorb neutrons and a proposed drug delivery system involving the use of an external magnetic field to direct the nanoparticles to targeted cancer sites. Boron nanoparticles were magnetically functionalized by encapsulating with an iron oxide shell. As such the exact composition, size distribution and oxidation states of the core/shell structures can affect treatment efficacy. Characterization is being done by electron energy loss spectroscopy (EELS) and x-ray energy dispersive spectroscopy (XEDS) within the electron microscope. Magnetic and additional electronic characterizations of the iron-oxide nanoparticles were performed by Mössbauer spectroscopy, whose results were compared with those of EELS Fe L_{23} peak ratio and a recent literature [1]. Both initial EELS and Mössbauer spectroscopy results show a mixed valence state, indicative of Fe_3O_4, for the iron-oxide nanoparticles.

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C-10

Total Tomography of III-As Nanowire Emitters: Correlating Composition, Strain, Polytypes, and Properties

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Ternary III-As nanowires (NWs) offer high efficiency, tunable emission and allow for direct growth on current Si CMOS technology, making them ideal as nanoscale emitters and detectors for on-chip photonic communications. In particular, (In,Ga)As quantum well (QW) shells grown on GaAs NW cores can emit in the near-IR by tuning the QW composition and diameter. In this work, we characterize (In,Ga)As/GaAs QW heterostructures that exhibit a blue-shifted emission near the top of the NW measured by spatially resolved cathodoluminescence (CL). As we aim to produce efficient, uniform emitters, it is necessary to understand the nature of this emission variation.

Electron backscattering diffraction and nano-probe x-ray diffraction measurements (performed at 26-ID-C of APS/CNM) reveal an extended segment of the polytypic wurtzite (WZ) structure embedded in the zincblende (ZB) NW. Direct correlation with CL shows an alignment between the blue-shifted region and the WZ segment. Nanodiffraction also probed strain along the length of the QW in correlation with structural mapping by scanning three Bragg conditions on the same wire. CL measurements were performed on the same wires after x-ray measurements to directly correlated emission and strain. FEM simulations match well with the experimental results, revealing minimal strain variations between the QWs in the WZ and ZB regions. Atom probe tomography (APT) was also used to map the composition of these structures in 3D. APT revealed a decrease in In mole fraction in the WZ region by about 4.5%. These measurements of morphology, composition, structure, and strain were combined as input for k p calculations of the QW band structure that reveal an emission shift between

the WZ and ZB of about 95 meV, matching reasonably well to the CL results giving a 75–80 meV shift. Ultimately, this correlative analysis allowed us to deconvolve the complex emission behavior of this NW QW heterostructure.

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C-11

Structural Changes of Layered Optical Nanocomposites as a Function of Pulsed Laser Deposition Conditions

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We developed a series of multilayer nanocomposite thin films consisting of $BaCl_2$ nanoparticle layers and optical dopants sandwiched between SiO_2 glass matrix layers. The films have potential optical applications including up- and down-convertors in photovoltaics. As the size, distribution and crystal phase of $BaCl_2$ particles affects the optical properties of the nanocomposites [1,2], it is very important to control these parameters and understand the effects of deposition conditions on the thin film structure. We therefore varied the pulsed laser deposition (PLD) conditions, used transmission electron microscopy (TEM) and energy-dispersive x-ray spectroscopy (EDS) analysis to determine the structure and composition of the thin films, especially of the $BaCl_2$ particles, as a function of deposition conditions. The samples were deposited on carbon membranes on TEM grids for plan-view analysis.

By adjusting the energy fluence and the $BaCl_2$ pulses, discrete, amorphous $BaCl_2$ nanoparticles were observed using plan-view TEM, which is what we are needing because crystallization can then be used to control optical behavior. The area covered by the $BaCl_2$ particles and their size both decreased by reducing laser energy fluence or the number of $BaCl_2$ pulses, though the in-plane shape of $BaCl_2$ particles remain roughly circular. The presence of these small circular $BaCl_2$ nanoparticles indicates that the growth mode of $BaCl_2$ on SiO_2 is a 3D island growth. However, under all deposition conditions used, we also observed very large circular $BaCl_2$ particles (up to micrometer size) which we believe are caused by condensed droplets from the locally melted target, and we are working to avoid these by adjusting the PLD parameters further.

JEOL 2100F TEM, Hitachi S-4700-II HR-SEM, Zeiss NVision FIB-SEM, FIB FEI Nova 600 NanoLab, Temescal FC2000 E-Beam Evaporator.

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C-12

Operando TEM Investigation of Sintering Kinetics of Nanocatalysts on MoS_2 in Hydrogen Environment

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The possibility of synthesis and scale-up of two-dimensional (2D) materials enable design of novel heterostructures for wide applications. Among the 2D family, transition-metal dichalcogenides like MoS_2 is of great interests in catalyst field since its excellent hydrogen evolution reaction (HER) activity as well as good thermal and chemical stability [1]. The heterostructure of MoS_2 combined with significant reduced amount of Pt is shown to have very exciting electrocatalytic activity [2]. However, degradation of nanocatalyst due to sintering decrease the active surface area resulting in a loss of catalytic activity strongly limits the application scope. Such degradation process of Pt on MoS_2, as well as methods to slow it down is not well studied and remains unclear. To investigate

the thermal behavior of nanocatalyst in real working conditions, we utilized *in situ* technique involving gas flow TEM to observe the sintering process under elevated temperature in combination with 1 atm H_2 gas environment. The Pt and Au@Pt nanocatlayst on MoS_2 were first synthesized by wet chemical reduction method and transferred onto Si microchips with SiN viewing windows. HAADF-STEM imaging combined with FFT, EDS and EELS mapping confirm the existence of Au core and a thin Pt shell on MoS_2 substrate.

To capture the sintering behavior of Pt and Au@Pt, a gas flow TEM holder was assembled with two microchips isolated to form a flow cell environment. H_2 gas was introduced into the cell with a constant flow rate and after that local heating was triggered in the sample area. The temperature was increased from room temperature (RT) to 400°C in 1.5 hr. TEM images were acquired after every 50°C increment. The electron beam was blocked at all time except initial TEM alignment and during imaging period. By comparing the starting and ending morphology of Pt nanoparticles at RT and 400°C in H_2 environment, a strong diffusion of smaller Pt towards the center larger Pt particle is observed, while the (200) surface orientation of center Pt remains unchanged. Example of three Pt particles coalescing behavior in H_2 as temperature increased from RT to 400°C are investigated and corresponding FFT show a change in both (200) and (111) surface orientations of these Pt particles, suggest that rotational movements of Pt particles are accompanied with diffusion behavior on MoS_2 (001) surface. In comparison, Au@Pt core-shell structures remain relatively stable with much less diffusion and rotational dynamics. These findings indicate that Au@Pt core-shell structure has better thermal stability compare to Pt nanoparticles on MoS_2 in H_2 environment at temperature of up to 400°C. This work presents an applicable way to gain atomic-scale information of supported nanocatalysts behaviors at standard pressure, and help provide insights into design of novel catalysts that are robust to high temperature working conditions.

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C-13

Manipulation of Spin Wave Propagation in a Magnetic Microstripe via Mode Interference

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Spin waves (SWs) are promising for high frequency information processing and transmission at the nanoscale. The manipulation of propagating SWs in nanostructured waveguides for novel functionality, has become recently an increased focus of research [1]. In this work, we study by using a combination of micro-focused Brillouin light scattering (μ-BLS) imaging and micro magnetic simulations the manipulation of propagating SWs in yttrium iron garnet (YIG) stripes via mode interference between odd and even modes. Due to the lateral confinement in a microstripe the SW spectrum (dispersion relation) is dominated by a set of hybridized symmetric odd SW modes causing a self-focusing effect [2]. The situation changes, when the externally applied magnetic field in the sample plane is locally varied by the magnetic stray field of a nanopatterned permalloy (Py) dot in proximity to the YIG wave guide. This can lead to a symmetry breaking, causing an excitation of antisymmetric even SW modes. Through varying the position of the Py dot along the stripe, which corresponds to varying the phase difference between the odd and even modes, the channels for the propagation of SWs can be controlled. These results show a new method to excite and control asymmetrical even SW modes. This opens new perspectives for the design of magnonic devices with novel functions.

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Nanoscience and Nanotechnology

C-14

Light-gated Synthetic Protocells for Plasmon-enhanced Solar Energy Conversion

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Engineering of synthetic protocells with man-made compartments to reproduce specific cellular functions has received significant attention in fields ranging from origins-of-life research to synthetic biology and biomedical sciences [1,2]. Inspired by the hydrothermal-vent origin-of-life hypothesis that prebiotic syntheses were confined and catalyzed by compartment-like iron monosulfide precipitates, synthetic protocells constructed with inorganic nanoparticle-packed colloidosomes have recently been put forward as an alternative primitive paradigm [1]. To recreate synthetic protocells mirroring the phase when protocells relied on both inorganic walls and organic membranes to orchestrate protometabolic reactions, we constructed a light-gated protocell model made of plasmonic colloidosomes assembled with purple membranes for converting solar energy into electrochemical gradients to drive the synthesis of energy-storage molecules [3]. This synthetic protocell incorporated an important intrinsic property of noble metal colloidal particles, namely, plasmonic resonance. In particular, the near-field coupling between adjacent metal nanoparticles gave rise to strongly localized electric fields and resulted in a broad absorption in the whole visible spectra, which in turn promoted the flux of photons to the sole protein of purple membrane, bacteriorhodopsin, and accelerated the proton pumping kinetics. The cell-like potential of this design was further demonstrated by leveraging the outward pumped protons as “chemical signals” for triggering ATP biosynthesis in a coexistent synthetic protocell population. In this way, we lay the ground work for the engineering of colloidal supraparticle-based synthetic protocells with higher-order functionalities for different applications such as solar energy conversion.

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C-15

On the Homogeneity of TiN Kinetic Inductance Detectors Produced through Atomic Layer Deposition

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We report on the homogeneity of a TiN thin film deposited on silicon wafer using atomic layer deposition (ALD). The critical temperatures, T_C, of four identical microwave kinetic inductance detectors (MKIDs) fabricated in this film are measured. The value of T_C is invariant for MKIDs belonging to the same fabrication process. However, we observe the resonance frequency, kinetic inductance, and quality factor exhibit a clear variation for each MKID (part of which may be attributed to the transmission line).

First, we show the design of the MKID, the resonators, and the CPW transmission line. In general, the process of fabrication of an MKID is presented. For example, the deposition was done with 300 layers via atomic layer deposition.

Second, we show the methods of characterization to obtain the resonance frequency and the loaded quality factor of a resonator. In addition, the method to obtain the critical temperature of each resonator is shown. This involves doing a fit of the fractional resonance frequency change as a function of the temperature.

Finally, the values of the critical temperature, resonance frequency, and loaded quality factor are shown. The variation in the critical temperature obtained by atomic layer deposition (0.5%) is smaller than variation seen when using sputtering (25%). However, the percent variation in the resonance frequency is higher than with sputtering [1,2]. As a consequence of those results, possible causes and solutions are discussed.

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C-16

Mask Free Patterning of Custom Inks for Controlled CVD Growth of Two-dimensional Crystalline MoS_2 and WS_2 Semiconductors

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Two-dimensional van der Waals semiconductors called transition metal dichalcogenides (TMDCs) have versatile properties, they are fundamentally and technologically interesting and hold promise for numerous applications; opto-electronics, energy storage, electrocatalysis, sensing and many more. Recently, various patterning approaches and synthesis methods have been utilized to produce these layered nanomaterials. We report here on a novel, low-cost and mask-free approach which enables controlled selective growth of molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) crystalline islands on Si/SiO_2 substrates [1]. In particular, the direct-write patterning (DWP) technique and chemical vapor deposition (CVD) method are employed to produce arrays of 2D-TMDCs nanostructures, at pre-defined locations on the Si/SiO_2 substrates. It is shown that by tuning the patterning parameters, the inks composition, concentrations of ink-precursors, and the growth conditions specific MoS_2 and WS_2 nanostructures with controlled morphology, could be produced. As grown materials were analyzed by atomic force microscopy, Raman spectroscopy, transmission electron microscopy, and x-ray photoelectron spectroscopy, which confirmed a quality double-layer MoS_2 and WS_2 nanostructures. The field effect mobility values of 11 $cm^2/V\text{-}s$ for MoS_2 and 4 $cm^2/V\text{-}s$ for WS_2 were extracted from the electrical measurements performed on back-gated field effect transistors.

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C-17

Folding, Self-assembly and Characterization of Giant Metallo-supramolecules with Atomic Resolution

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Nature extensively utilizes folding and self-assembly to construct various protein systems. Inspired by Nature, we herein designed and synthesized metal-organic ligand with specific sequence of terpyridines installed. Through adding different equivalents of metal ions, we built a discrete metallo-supramolecule on the basis of intramolecular and intramolecular complexation with diameter > 20 nm and molecular weight 65785Da. Such giant supramolecular architecture with 13 hexagons is among the largest metallo-supramolecules ever reported. As such the characterization became extremely challenging given the size, shape and disordered subdomain. In the first level of characterization, mass spectrometry and NMR were used to monitor the folding and self-assembly process. After that, ultrahigh-vacuum low-temperature scanning tunneling microscopy (UHV-LT-STM) was able to visualize each coordination unit with atomic resolution. More importantly, with the investigation of point spectroscopy on each metal atom, we were able to characterize the disorder subdomain and identify the isomeric structures.

C-18

Optimizing the Design of Tapered X-ray Fesnel Zone Plates Using Multislice Simulations

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Alcorix Co. is currently developing a batch fabrication method for hard x-ray fresnel zone plates (FZPs) based on atomic layer deposition of multilayer, nanolaminate films surrounding a central silicon pillar [1]. Since these FZPs will operate at high x-ray energies (12 keV to 100 keV), the Fresnel zones must be at least several microns thick to induce the necessary phase shift in the x-ray wavefront. Additionally, the zones must be tapered so that the x-rays fulfill the Bragg diffraction condition as well as possible. In order to guide our experimental design, we have performed volumetric simulations of FZPs using multislice scalar wave propagation.

Multislice simulations enable volumetric simulations of thick x-ray FZPs and other x-ray optics [2]. We have produced multislice simulations that calculate parameters such as optimal taper angle at several focal orders. From analysis of how the taper angle affects the x-ray intensity at different focal orders, we have determined a set of optimal parameters for our first generation prototype FZPs. In this poster we will show how various simulation conditions (e.g., grid density, number of slices) affect the results. We will also show how precise control of the taper angle is crucial for optimal FZP performance and how we are gaining experimental control over this important parameter with Bosch etching of Si.

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C-19

Random Sampling of Ionic Radii and Discrete Distributions for Structural Stability and Formability of Titanium-based Perovskites

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Titanium-based perovskites are highly stable semiconductors in humid and/or hot environments with tunable bandgaps (1.5 ~ 2.43 eV) suitable for photovoltaics and photoluminescence applications. Recent studies show that Titanium (Ti) metal is a promising candidate as a metal cation in forming stable perovskites (A_2TiX_6 and/or $ATiX_3$) replacing their conventional toxic Pb- based counterparts; where A refers to an organic and/or inorganic cation (e.g., Cs^+, MA^+, and Rb^+) and X is a halide anion (e.g., F^-, Cl^-, Br^- and I^-). Here, we theoretically investigate on the formability and stability of various Ti-based perovskites relying on a random sampling of reported ionic radii (e.g., Shannon, Pauling, and Stern) for determining perovskites structural maps from Goldschmidt's tolerance factor (t) and octahedral factor (μ). Twelve Ti-perovskites are chosen by mix/match of the given cations and anions. Probabilities of formation are estimated from normal and binomial distributions of random samples based on desired outcomes, mean, and standard deviation. Results revealed that $Cs_2Ti\text{-}X_6$ and $RbTi\text{-}X_3$ are stable (formable) with all halogens except for I^- with only ~0.5 formation probability of Cs_2TiI_6 and $RbTiI_3$ samples due to large anion radius (I^-~2 Å → overlapping) preventing Ti atoms from occupying B-sites in the octahedral. $MATi\text{-}X_3$ is more controversial with more formation tendency for $MATiCl_3$ and $MATiBr_3$ (>0.8) as compared to their counterparts (<0.5).

C-20

Fabrication of High-aspect-ratio Gold-in-silicon X-ray Gratings

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Hard x-ray phase-contrast imaging is a promising approach for improving soft-tissue contrast and lowering radiation dose in biomedical applications. The method key components are high-aspect-ratio gold-in-silicon gratings with sub-micrometer periodicity. The quality of gratings strongly affect the quality of the generated images. Fabrication of high-aspect-ratio high-resolution dense nanostructures is challenging, and limits hard x-ray phase-contrast imaging practical implementation. To fabricate the gratings, two key technological challenges must be addressed: (i) creating a high-aspect-ratio trenches with smooth vertical walls, and (ii) filling the trenches uniformly with gold.

We report our progress in fabrication of 450 nm half-pitch gold gratings with an aspect ratio of 27 using laser interference lithography (LIL), reactive etching (RIE), atomic layer deposition (ALD), and gold electroplating techniques. The gratings area is 30 mm long and 15 mm wide. In the first step, gratings were patterned on the resist/chromium coated silicon wafer *via* LIL. Then, chromium, which served as a hard mask for the silicon etching, was etched using RIE. This step was followed by cryogenic RIE to create deep trenches in silicon, and a platinum seed layer deposition by ALD. Finally, the trenches were filled with gold using conformal electroplating, when plating occurred from all surfaces.

The demonstrated capability provides valuable information for the fabrication of large area high-aspect-ratio nanometric periodic structures.

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C-21

Fluid-based Capillary Compound Refractive Lenses for X-ray Free Electron Lasers

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X-ray free electron lasers offer unprecedented intensity of fully coherent x-rays for various scientific investigations. An unfortunate consequence of this large intensity is that the x-ray beam causes radiation damage both to the sample as well as any optics that are placed in the beam path. As a result, scientists have developed techniques such as single-shot imaging that collects as much information in a single x-ray pulse before the sample is destroyed. With a similar goal in mind, Alcorix Co. has begun developing prototypes for “single-shot” compound refractive lenses. These lenses are formed out of a constantly replenishing array of bubbles inside of an open-ended capillary tube. As each x-ray pulse travels through the tube the bubbles that are present at the time inside of the tube will focus it. Before the next x-ray pulse arrives, a similar configuration of bubbles will be introduced into the tube.

In this poster, we will describe the operating principles of this open-ended capillary tube and will show the current status of our prototype development. Additionally, we will show our progress with controlling the shape of the meniscus of the bubbles inside the tube as well as calculations for focusing properties with different fluids. The ultimate goal of this project is to have a viable focusing system for XFELs.

C-22

Engineering Nano-biocomposite Materials Using CNTs and ZnO Hybrid Interfaces and Hydrogel Environments for Future Biomedical Applications

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One dimensional (1D) nanoscale objects such as carbon nanotubes or other nanowires represent a unique opportunity for utilizing their large surface area and high aspect ratio. Therefore,1D nanowires can be functionalized through their entire length with specific biological molecules or other nanoscale moieties via covalent bonding, physisorption or chemisorption. 1D nanowires with diameters of 1–5 nm, in carbon nanotubes (CNTs), and 50–100 nm in zinc oxide nanowires (ZnO NW),have been produced in a controlled fashion [2]. They are great candidates for biomedical applications, due to unique morphological, electronic properties and biocompatibility. For example, they provide nano-textured surface for molecular immobilization, enhance electrical conductivity in the composite materials, when incorporated into nonconductive environments, could improve the mechanical strength of composite materials and be used as power lines for transmitting electrical signals to biological cell for stimulation/recording. The goal here is to investigate the use of CNTs and ZnO NW in composite biomaterials and as hybrid new platforms for future biomedical applications.

In this work we investigate single-walled (sw)-CNTs and multi-walled (mw)-CNTs as well as ZnO NWs and CNTs/ZnO composite hybrid structures as surfaces that could interface with other biomaterials such as hydrogels.The sw-CNTs/hydrogels interfaces have demonstrated great potential in facilitating healthy neuronal cell behaviors, such as cell attachment, proliferation and neurite growth [1]. Designing new ZnO/Hydrogel and CNTs/ZnO/Hydrogel composites could expand medicinal benefits of these nano-biomaterials in targeting multiple medically important questions including but not limited to neural cell regeneration, cancer treatments and drug delivery.

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C-23

Characterization of 3D Printed Lab on Chip Structures for Cell Culture Applications

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3D printing has recently been used extensively in a large number of applications due to its ability to make complex structures with ease compared to other conventional additive/subtractive methods. 3D printing of stents to bio-chips has become quite attractive for *in vivo* and *in vitro* applications respectively in biomedical applications. However, this requires a lot of research to ensure that the 3D printed surface is bio compatible and facilitate cell/tissue/organ growth in given conditions. In this study, we 3D printed polylactic acid (PLA) and acronitrile butadiene styrene (ABS) polymers with sandwiched glass structures for lab on chip application.

The 3D printed PLA and ABS surfaces were modified using hydrolysis (wet chemical etching) and UV/ozone techniques. The wettability of the surfaces were studied using contact angle measurement in as-printed and polished conditions. Surface modification by these techniques resulted in activation of –COOH groups for further radical attachment [1]. As a follow-up step, 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC) crosslinking technique was used to introduce primary amine to carboxylic groups which is ideal choice for cell culture [2]. These samples were studied using florescence measurements and UV spectroscopy which provided clear evidence that hydrolyzed samples show better protein attachment. These results were further verified using Raman spectroscopy to confirm protein attachment.

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C-24

Applications of Sequential Infiltration Synthesis (SIS) to Structural and Optical Modifications of 2-photon Stereolithographically Defined Microstructures

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Sequential infiltration synthesis (SIS) allows for permeation of phot-definable polymers, such as negative photoresists, with metal oxides, which dramatically alters the mechanical and optical properties of the underlying structures. In this work, we show how SIS affects the properties of 3D structures created using the process of 2-photon stereolithography. The significant changes, both from a mechanical and optical perspective, enable a suite of tantalizing applications in the field of photonics, microrobotics, sensing, and bio-compatible materials. In particular, we show how the infusion, combined with morphological designs of the internal 3D scaffolding, allows for complete permeation of SIS into the material. We also show how such permeation, together with a 3D optical properties of an artificial photonic crystals can be utilized to achieve highly selective sensing of environmentally related gasses, such as methane. In addition, we show the applications of this technology to wireless power transfer of untethered MEMS microfliers, which are the smallest artificial flying structures currently in existence.

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C-25

Temperature Dependent Skyrmion Hall Angle in Ferrimagnets

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Analogous to the Hall effect where electronic charges moving in the presence of a magnetic field acquire a transverse velocity, magnetic solitons with non-zero topological charges (i.e., skyrmions and chiral domains walls) exhibit the skyrmion Hall effect [1], which opens up new possibilities for manipulating

the trajectories of these quasiparticles. The skyrmion Hall effect has been theoretically predicted to vanish for antiferromagnetic skyrmions because of the cancelation of opposite topological charges [2] and experimentally demonstrated to vanish in ferrimagnets at the compensation temperature [3]. We present a study of current driven domain wall dynamics in artificially ferrimagnetic multilayers: Ta(4 nm)/Pt (5 nm)/[Co (0.5 nm)/Gd (1 nm)/Pt(1 nm)]$_{10}$/Al (2 nm). The magnetic texture in different layers of the multilayer films are coherent and antiferromagnetically aligned. Here we experimentally investigate the temperature dependence of the current driven magnetization dynamics from room temperature down to temperatures below the compensation point at around 100 K and show a dependency of the skyrmion Hall angle on the applied temperature.

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C-26
Selectivity through Morphology: Towards Highly Sensitive MOX/CNT Based Hydrocarbon VOC Sensors

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Bare carbon nanotubes (CNTs) are insensitive towards most gases due to poor bonding between the chemically inert graphitic surface and different compounds they are exposed to. Consequently, for gas sensing applications, functionalization of CNTs with reactive compounds is required. By introducing surface pre-treatments prior to functionalization, the affinity of the functionalizing species is enhanced, enabling the fabrication of highly sensitive CNT chemiresistor-based sensors.

Atomic layer deposition (ALD) allows precise, uniform and conformal deposition of oxide coatings on geometrically complex substrates such as MWCNTs [1]; thus offering a suitable route for the functionalization of MWCNTs for gas sensing applications. In this work, we show how the morphology of ALD-deposited metaloxide (MOX) nanocrystals (NCs) interacts with the chemical structure of certain VOCs, such as toluene or xylene to produce strong signal specific to these target VOCs. We show that MWCNTs are p-type semiconductive, a property that enhances the sensing mechanism. In contrast to other VOC sensors, the proposed sensing mechanism has low sensitivity to other VOCs, such as formaldehyde and benzene, and is specifically selective to dimethylbenzenes. We demonstrate the use of this method to achieve reliable ppm-level detection of toluene at room temperature.

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C-27
Direct Grain Boundary Study in Cerium Oxide

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Charge transport across and along grain boundaries can have profound implications on the macroscopic behavior of materials used in solid oxide fuel cells, batteries as well as other energy technologies. The grain boundary may serve as high conductivity pathway or roadblock for ionic or electronic carriers. Even pristine grain boundaries, free of secondary phases, can display modified transport properties relative to the bulk as a result of space charge effects. This is particularly true of doped ceria, which is a leading candidate for a range of applications due to fast oxygen ion conduction in the bulk. To date, the vast majority of grain boundary studies have relied on macroscopic measurements that yield ensemble averages [1]. However, a fundamental understanding of their behavior requires access to the properties of

individual grain boundaries, in terms of both chemistry and electrical profiles. Electron holography offers an excellent combination of high spatial resolution and sensitivity to measure mean inner potential as well as grain boundary potential in these materials.

The goal of our work is to perform direct measurement of the inner potential in the grain boundary region of 0.2% Sm-doped Ceria (SDC02) using electron holography. The ceria sample was synthesized by using high purity starting powder Cerium Oxide (99.995%, Sigma-Aldrich) and Samarium Oxide(99.999% Sigma-Aldrich). It was prepared by pressing and sintering at 1500°C for 10 hours and followed by standard TEM specimen preparation techniques of polishing and Ar ion milling. We performed electron holography on the grain boundary region of as-prepared polycrystalline ceria during an in-situ heating experiment where the sample was heated to 300°C. The off-axis electron holography was performed using Tecnai F20 TEM at the Center for Nanoscale Materials at Argonne National Laboratory. The holography experiments were performed with a biprism bias of 100V which yielded a good fringe contrast (>30%) and spatial resolution(0.6 nm). Diffraction contrast was carefully reduced by tilting the grains away from the zone axis [2]. The grain boundary potential was calculated from the measured phase shift of the electrons by accounting for the thickness of the sample.

Generalized Mott-Schottky model by including charge density in GB core were proposed to understand the origin of grain boundary potential. The charge transport measurements using AC impedance spectroscopy [3] on the same batch of ceria sample combined with fitting results from the model were found to agree well with the holography results. We were able to confirm that the as-measured GB barrier potential and width were indeed related to the space charge potential and space charge layer thickness. We investigated different types of grain boundaries with varying misorientation, and the results showed that grain boundaries with higher misorientation angle about [110] axis showed larger potential. We additionally performed atom probe tomography to determine the causes for the larger grain boundary potential measured. Impurities were found segregated in the GB core which matched well with the charge density level predicted by our proposed model. This study showed that electron holography can be successfully used for measuring space charge effect at the grain boundaries in ionic conductors such as ceria. More importantly, the role of impurity in GB core was found to be the main cause for the space charge effect in polycrystalline cerium oxide samples.

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ESRP POSTER ABSTRACTS

ESRP-1

Local Structural Studies of Pd Based Catalytic Nanoparticles

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The purpose of this experiment will focus on the study of the atomic organization of nanoparticles of palladium, palladium/copper, palladium/cobalt, and palladium/nickel. The nanoparticles' structure are studied using extended x-ray absorption fine structure (EXAFS). X-ray absorption spectroscopy measurements are performed on both edges of the nanoparticles. This allows us to determine the arrangement of the metals within the nanoparticle. Due to their reduction in size and increase in surface area, bi-metallic nanoparticles (BNPs) are prominently used as catalysts. BNPs have proven to be the best performing catalysts for fuel cell oxidation processes. One of the major problems in understanding how these nanoparticles function is to have a clear picture of their structure. X-ray absorption spectroscopy provides local structural information, which can be used to distinguish core-shell atomic distributions from uniformly alloyed distributions. This kind of structural understanding, combined with the catalytic properties, can help design better catalysts for the future [1,2].

Thank you to Elena Timofeeva for helping us to prepare samples for study at IIT. Thank you to John Katsoudas for the in-depth explanation of the beam process. Thank you to Carlo Segre for his mentorship with the students of Bolingbrook High School throughout this entire experience.

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ESRP-2

The Characterization of Phytochelatins Mediating Zinc Transport in *Arabidopsis thaliana*

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Zinc is an essential microelement involved in multiple higher plant processes that require enzymatic cofactors for function. Both excess and deficient levels of zinc are problematic for higher plants. The homeostasis of zinc in higher plants involves a complex interaction of responses to environmental stimuli and regulation by multiple genes resulting in efflux, sequestration and chelation of zinc [2,4]. It is desirable to more fully understand the complex nature of zinc homeostasis due to current increase in anthropogenic activities that contribute to toxicity or deficiency in soils which leads to food insecurity. Ionomics as a means to characterize phenotypes of mutant plants has led to a greater understanding of complex nature of gene functions that code for the regulation of microelements. Synchrotron xrf allows for increased resolution and detection of these microelements without seed preparation that can potentially affect tissue integrity [3]. One mechanism of Zn homeostasis that is of interest involves the production of phytochelatin synthase (At PCS 1) which produces phytochelatins (PC) as a feedback response to environmental zinc levels. It has been hypothesized that Zn-PC chelated complexes may be involved with the translocation of Zn [1]. This study used Syncrotron X-ray fluorescence (SXRF) and microtomography to evaluate microelement speciation, placement and relative concentration in *A. thaliana* wild type Col-0 versus PC-deficient mutant *cad* 1-3 seed. Differences in whole seed Zn concentration as measured by sxrf (counts per pixel) suggest that the translocation of Zn-PC complexes to seed is affected. Whole wild type Col-0 seed concentrations were twice that of mutant *cad* 1-3 seed. Unanticipated increased embryonic vascular tissue Fe deposition were detected. Microtomography results do not suggest variation in wild type versus mutant seed microelement deposition patterns.

Thanks to ABRC for A. thaliana seed. This research was made possible through the Exemplary Student Research Program, supported by Argonne National Laboratory's educational programs, GSECARS and the University of Chicago and the Advanced Photon Source (APS), Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

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ESRP-3

Local Structure Analysis of Chromophore $YGa_{1-x}Mn_xO_3$

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This experiment investigates the local environment around Ga^{3+} and Mn^{3+} ions in $YGa_{1-x}Mn_xO_3$ chromophores. We explore the structural origins of this chromophore's visible purple hue variations that can be formed over a range of small values of x. Such understanding may lead to applications of this inorganic oxide material being used as a non-toxic pigments suitable for applications in paints and dyes. While x-ray diffraction results provide an average description of the trigonal bipyramidal units about Ga/Mn atoms with five oxygens surrounding the cation, the x-ray absorption near edge structure of these materials may allow us to investigate the structural causes of these shades of purple. As such, these processes will be used to study both the large scale and local structure of this chromophore.

We would like to share our sincere appreciation to Dr. Segre who provided his invaluable support in this experiment and in the richness of our experience. In addition to leading us in this experiment at Argonne, he traveled to Glenbrook South High School numerous times. Dr. Segre shared his time, expertise, and passion for understanding the nature of materials. We are very, very grateful.

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ESRP-4

Examining the Crystallization of Gold Nanoparticles Based on Variable Surface Pressure

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Nanoparticle films have a wide range of applications that include sensors, transistors, photovoltaic cells, and filtration devices; however, their self-assembly is still being explored. Nanoparticle films have unique properties that include superparamagnetism, surface plasmon resonance, and quantum confinement. Analyzing the properties of self-assembled nanoparticle films and tunable nanoscale crystal structures will open mankind to a series of inventions and innovations in the fields of materials science and nanoelectronics. In previous experiments with Lead (II) Sulfide nanoparticles, our team has observed that the type of ligands as well as their surface density can alter interparticle spacing. The aim of these experiments was to analyze the three-dimensional structure of the crystallized nanoparticles. This year, however, the ligand type and surface density will remain constant using Gold nanoparticles. Our objective is to observe the changes between the two-dimensional and three-dimensional structures of nanoparticles during crystallization by varying the surface pressure and presence of additional ligands. The change in pressure will cause an increase in particle interactions. This will cause the monolayers to form multilayers and thus the crystal structure. Hence, the specific goal of this research is to ascertain the direct structure of Gold nanoparticles in two-dimensions.

ESRP-5

Root Uptake of Chromium and Nickel in Common Plants and Vegetables

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The presence of cadmium, selenium, nickel, chromium, and arsenic in Asian and Canadian soil samples recently drew the attention of federal food and drug administration agencies as well as the World Health Organization due to the toxicity these elements produce. Excessive exposure to nickel is associated with severe stomach aches, increased red blood cells, and increased proteins present in urine. Exposure to chromium is linked to decreased hemoglobin content, decreased hematocrit content, and increased total white blood cell counts reticulocyte counts, and plasma hemoglobin in humans. These elements contaminate and harm plant life--therefore increasing unsustainability in local ecosystems. Through Lemont High School's Exemplary Student Research Program (2018–2019), students will work closely with Dr. Olga Antipova (Argonne National Laboratory), Olena Ponomarenko (University of Saskatoon), and Shengke Tian (Zhejiang University, China) to examine the relationship between the contamination of these plants with heavy metals and their root uptake with a focus on nickel and chromium. Our student group

will participate in testing, observation, and analysis of plant uptake of chromium and nickel to determine the long-term impacts of element toxicity and its relation to plant vitality. It's essential to understand the allowance of these elements in ground-rooted plants to produce a high confidence level to regulate these elements in consumer products.

Thank you to the Exemplary Student Research Program, supported by Argonne National Laboratory's Educational Programs (CEPA), the APS User Office, Dr. Olga Antipova, and Lemont High School teacher Erin Horan. Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

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ESRP-6

Study of Ferrous Sulfate Oxidation under Extreme Conditions Using X-ray Absorption Spectroscopy

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The purpose of this experiment is to analyze how various factors affect the rate of the oxidation of ferrous sulfate into ferric sulfate in iron supplements. The experiment will involve exposing samples of iron supplements to oxygen and heat over varying lengths of time. The experiment is expected to reveal the extent to which exposure to heat and oxygen affects the oxidation rate of ferrous sulfate. The experiment will utilize the APS by employing the XANES and EXAFS methods. This x-ray absorption spectroscopy will produce data that shows the oxidation state of the present iron along with the local coordination environment. The results are anticipated to show an increase in the amount of Fe^{3+} present in the samples exposed to heat and oxygen when compared to a control [1].

Thank you to Dr. Tianpin Wu for her work outside our visit in preparing samples and collecting further data. She invested her time to guide us through data collection and analysis and imparted invaluable wisdom to the entire team.

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ESRP-7

Optimizing Data Collection at Beamline 17-ID Using Bovine Insulin

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Beamline 17-ID is operated by IMCA-CAT, a collection of pharmaceutical companies, to analyze samples for drug discovery. The beamline 17-ID is unique, and thus attempting to optimize the beamline's settings may improve beamline research and exposure by increasing its efficiency for all those who use it. The student researchers proposed to provide other beamline users with statistical data of preset data collection settings that would help them understand the parameters of beamline 17-ID. This would potentially reduce the time that is needed to shoot their samples; therefore, beamline users' time would be more cost-effective. The statistical data collected by the students on the beamline 17-ID may be used as a starting point for the testing of samples with similar characteristics to bovine insulin. The data collected and analyzed last year using Rmerge values suggested that a more in-depth study over a smaller range of exposure times would be beneficial. This year, the students focused in on a narrow range of exposure times that were highlighted from last year's data.

Erica Duguid; IMCA-CAT, Hauptman Woodward Medical Research Institute, Sector 17. The team would like to thank Dr. Duguid for her continued patience and counsel when collecting and analyzing crystal samples. Her enthusiasm and guidance were essential to introducing the team to the excitement of crystallography.

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ESRP-8

Copper Oxidation States Found in Wood Preservatives and Their Relationship to Corrosion Factors

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Wood preservatives containing metals are widely used for wood protection in residential construction. Preservative systems typically contain copper in various forms paired with organic co-biocides. Past research has indicated that the predominant form of copper found in preservative treated wood is Cu+2, but recent x-ray absorption experiments of wood in contact with aged corroded fasteners indicate Cu+1 is the predominant form within the cell wall. There are distinct differences between Cu+1 and Cu+2 with respect to their solubility and biological activity against microbes. The goals of these experiments are to characterize Cu valence states in various commercially available wood preservative treatment formulations in order to fill a long standing knowledge gap and establish an improved conceptual model for both wood preservative metal speciation and the initiation of wood decay.

ESRP-9

Study of Industrial Metals in Soils Collected from Chicago Residential Areas

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X-ray fluorescence was used to estimate the concentration of potentially toxic metals in various soil samples. Soil was taken from separate locations in the city of Chicago which are in the vicinity of industrial activities involving metals. A background soil sample was also taken at a location in Saint Charles, Illinois away from suspected industrial use of metals. Fluorescence yield scans were taken for each of the samples at DND-CAT's station 5BMD, and x-ray absorption near edge structure (XANES) scans were collected on a subset of samples to compare and contrast the types of metal compounds present.

Portions of this work were performed at the DuPont-Northwestern-Dow Collaborative Access Team (DND-CAT) located at Sector 5 of the Advanced Photon Source (APS). DND-CAT is supported by Northwestern University, E.I. DuPont de Nemours & Co., and the Dow Chemical Company. 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.

ESRP-10

Testing Graphene as a Protective Coating for $LiMnO_2$ Batteries

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This study aims to characterize structural degradation of a MnO_2 cathode in the presence and absence of a graphene coating. $LiMnO_2$ has potentially high capacity due to its Li content and due absences of cobalt, it is less expensive and toxic than other cathode options; however, irreversible loss of oxygen surrounding the Mn atoms causes a rapid loss in capacity. There is evidence to suggest that the graphene coating will prevent the structural degradation of the cathode, resulting in higher capacity retention than has been observed with this cathode previously. For this experiment, $LiMnO_2$ batteries were created either with or without a graphene coating, then cycled through charge and discharge cycles to simulate use and test for capacity retention. After cycling, the cathodes were analyzed by XAFS to characterize structural degradation of bonds between neighboring atoms at the Mn edge.

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- Tip/Tilt Mirrors;
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- Piezo Motors, Piezo Drivers & Digital Motion Controllers;
- Voice Coil Actuators, MicroMotion Robots

Quantum Detectors
R104, RAL, Harwell Oxford
OX11 0QX
United Kingdom
Tel: +44 1235 445 795
http://quantumdetectors.com

Quantum Detectors has provided novel technology to the APS for several years, with the first installation of an Xspress 3 detector readout system here in 2014. Since then several more systems have been installed around the ring enabling higher throughput, wider dynamic range, and faster experiments.

As well as advanced detector readout systems we've also installed several MerlinX detectors at the APS. A 55µm energy resolving detector with up to eight thresholds in Colour Mode and employing a Medipix3 ASIC to achieve rates of 1200 Hz in 12-bit mode, MerlinX is a high-performance x-ray imaging detector that requires no supplementary cooling system. Additionally, we have Hexitec: A fully spectroscopic hard x-ray imaging detector which measures the energy and position of every incident photon in the 4-200 keV range. If you'd like to hear how we could provide better usability, enable faster throughput and in some cases offer a completely new mechanism for detection at your beamline, drop by our booth to learn more.

Rayonix, L.L.C.
1880 Oak Ave.
Suite 120
Evanston, IL 60201
Tel:847 869 1548
https://www.rayonix.com

Rayonix L.L.C. integrating Rayonix HS (High-Speed), now offer geometries for XFEL applications, that allow the direct beam to pass through the detector. Other new detector geometries allow SAXS to pass through in vacuum, for simultaneous SAXS/WAXS data collection.

Rayonix is developing a new ultra high speed pixel array X-ray detector with special features to support pump-probe experiments and 2-color experiments.

RaySpec
1 The Valley Centre
Gordon Road
High Wycombe, BKM
HP13 6EQ,
United Kingdom
https://www.rayspec.co.uk

Specialist design and manufacture of fluorescence detectors for synchrotron applications. RaySpec offers custom detectors designed to optimise geometries, efficiencies and performance on individual end-stations. Based on Silicon Drift Detector technology, RaySpec's detectors range from single sensor to multi-sensor assemblies with up to 19 individual channels. Specialities include focussed sensor arrays for optimum source-detector geometry, low energy windows (including windowless) and through-hole detectors for high solid-angle backward angle detection around the incident beam. RaySpec's SDD detectors may be used in air or in vacuum, with specialised UHV solutions available and they are designed for high rate operation with ASIC readout and 'next generation' DPP compatibility. To discuss your ideas and applications, please visit our booth and find out more about RaySpec's expertise and capabilities.

Rigaku Innovative Technologies, Inc.
1900 Taylor Road
Auburn Hills, MI 48326
Tel: 248-232-6400
https://www.RigakuOptics.com

RIT utilizes its staff of 10 PhD Scientists and 10 Engineers with over 250 years combined experience to provide the customer with the best solution to their coating and optics needs. RIT has provided optics and coatings to many of the world's synchrotron and free electron laser facilities with excellent results. While RIT specializes in reflective multilayer coatings for use in the VUV – Hard X-ray wavelengths, RIT can also provide single film and crystal optics for synchrotron and free electron laser beamlines and end stations. RIT's large deposition chambers allow for precise coatings to be applied to substrates up to 1.5 meters in length. Mirrors coated by RIT may also have multiple "stripes" allowing for different material systems or d-spacing designs on the same optic. This reduces the need for multiple optics, time consuming optic changes, and allowing for a wide range of energies and bandpass choices in the same optic. Rigaku Innovative Technologies also has developed a proprietary methodology for the complete refurbishment, recovery, and restoration of synchrotron and custom multilayer systems. These refurbished optics utilize the existing, often expensive, substrates allowing for lower costs and shorter lead times in replacing worn or damaged optics. Rigaku Innovative Technologies looks forward to continue to provide cutting edge X-ray and EUV optics technology to the world's premier synchrotron and free electron laser facilities.

SPECS-TII, Inc.
20 Cabot Blvd.
Suite 300
Mansfield, MA 02048
Tel: 508-618-1292
https://www.specs.com

SPECS leads the way in state-of-the-art technology, cutting-edge components, and compact and individually designed systems for surface analysis. The customized systems are highly integrated with facilities for sample and thin film preparation and in-situ analysis from UHV to high pressures. Our newest solution for environmental XPS is the award-winning EnviroESCA, which features quick sample throughput at Near Ambient Pressure. Our innovative product for ARPES research is the KREIOS 150, which combines a hemispherical analyzer with a new PEEM lens approach. This allows it to access the full photo electron emission hemisphere (±90°). We also offer a variety of sources for deposition, excitation, and charge neutralizers as well as analyzers, X-Ray sources, and research microscopes like LEEM and LT-STM.

Spellman High Voltage Electronics Corporation
475 Wireless Blvd.
Hauppauge, NY 11788
Tel: 631-630-3071
https://www.spellmanhv.com

Spellman High Voltage Electronics Corp is the world's leading independent supplier of precision DC high voltage power supplies, X-Ray generators and Monoblock® X-Ray sources for medical, industrial and scientific applications. While we offer the broadest and most advanced range of standard and platform products in the industry, we specialize in partnering with OEM's to develop, produce and support the optimum solution for each system and market segment. We advance medical care, industrial processes, quality control, scientific research, security and telecommunications by providing innovative high voltage power conversion solutions that enable equipment manufacturers to achieve their systems' performance, reliability, and cost goals. We currently have five design centers, six production centers, eight repair locations and over 2,200 employees in North America, Europe and Asia.

Starrett Tru-Stone Tech
1101 Prosper Drive
Waite Park, MN 56387
Tel: 250-251-7171
https://www.tru-stone.com

Starrett Tru-Stone Technologies specializes in precision granite machine bases & assemblies. We partner with you to add expertise in design collaboration, high-quality on-time manufacturing and complex assembly for your precision base. In addition to granite bases, Tru-Stone techs install precision rails, air mounts, brackets, pneumatic systems and cabling. Custom stands are also provided. Materials beyond granite include ceramic, carbon fiber materials.

Sydor Technologies
78 Schuyler Baldwin Drive
Fairport, NY 14450
Tel: 585-750-8578
https://SydorTechnologies.com

Sydor Technologies is a global provider of advanced x-ray detectors and diagnostic instrumentation for the energy, research, and defense industries. We manufacture complex measurement solutions for the world's most advanced applications. Our products are customized to each user's requirements. Our hard and soft x-ray detectors are engineered to provide the best sensitivity, across the widest dynamic range, and are optimized for use at modern and up-and-coming lightsources. Our x-ray Diamond Beam Position Monitors (DBPM) are available in a variety of packages for use in ambient to UHV environments. X-ray streak cameras and framing cameras are available to accompany our line of gated imagers and visible streak cameras. Established in 2004, Sydor Technologies is headquartered in Rochester, NY and now supplies systems and support in over 33 countries. For more information, please visit www.SydorTechnologies.com

Talend Inc.
800 Bridge Parkway Suite 200
Redwood, CA 94065
Tel: 310-686-0891
https://www.talend.com/

Talend, a leader in cloud integration solutions, puts more of the right data to work for your business, faster. Talend Cloud delivers a single platform for simple and complex data integration tasks across public, private, and hybrid cloud, as well as on-premises environments, and enables greater collaboration between IT and business teams. Combined with self-service solutions and hundreds of pre-built connectors from SaaS applications to cloud data warehouses, Talend allows you to cost-effectively meet the demands of ever-increasing data volumes, users, and use cases.

Almost 3,000 global enterprise customers have chosen Talend to put their data to work. More than a third of the Fortune 100 U.S. companies are Talend customers including GE, HP Inc., and Domino's. Talend has been recognized as a leader in its field by leading analyst firms and industry publications including Forbes, InfoWorld and SD Times.

Talend is Nasdaq listed (TLND) and based in Redwood City, California.

TDK-Lambda Americas
Programmable Power Division
405 Essex Road
Neptune, NJ 07753
Tel: 732-795-4100
https://www.us.tdk-lambda.com/HP

TDK-Lambda Americas, Inc.
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Tel: +1 732.922.9300 x 235 Fax: +1 732.922.1441
Email: bonnie.west@us.tdk-lambda.com
Website: www.us.tdk-lambda.com
TDK-Lambda Americas High Power Division is a manufacturer of Programmable, High Density Power Supplies located in Neptune, N.J.. The Genesys ™ series of Programmable Power Supplies has the highest density in power levels from 750W through 15KW with output ranges up to 1500V and 1,000A.
TDK-Lambda Genesys™ Series of Programmable Power Supplies has the highest density, making the Genesys™ Series the most complete set of platforms with identical user interfaces . Platforms include 750W, 1500W, 2.4KW, 3.3/5kW and 10/15kW Output. Outputs available range up to 600V and 1,000A. In addition to saving space, GenesysTM power supplies contain extensive standard features that provide a new level of performance and flexibility. An optional LXI Certified LAN interface provides flexible system integration and functionality.

Teledyne Princeton Instruments
3660 Quakerbridge Road
Trenton, NJ 08619
Tel: 609-587-9797
https://www.princetoninstruments.com

Princeton Instruments provides state-of-the-art CCD, sCMOS, ICCD, EMCCD, emICCD, X-Ray and InGaAs cameras; spectrometers; spectrographs; imaging systems; optics and coatings that are key to the success of your application. We take pride in partnering with our customers to solve their most challenging problems in unique, innovative ways.

Teledyne Signal Processing Devices Sweden AB
Teknikringen 6, SE-583 30
Tel: +46 13 465 06 00
https://spdevices.com/

Teledyne SP Devices designs and manufactures world-leading modular data acquisition and signal generation instruments. Our products utilize patented calibration logic, the latest data converters, and state-of-the-art FPGA technology resulting in an unrivaled combination of high sampling rate and resolution. Products are available with a range of application-specific features and embedded, real-time signal processing.

Toho Technology Inc.
4809 N. Ravenswood
Suite 113
Chicago, IL 60640
Tel: 773-5837183
http://www.tohotechnology.com/

Toho Technology Inc. provides Material Characterization solutions and Surface Metrology. Through a partnership with industry leader Nanometrics, Toho Technology now offers comprehensive metrology solutions used to monitor the physical, optical, electrical and material characteristics of compound semiconductor, strained silicon and silicon-on-insulator (SOI) devices, including composition, crystal structure, layer thickness, dopant concentration, contamination and electron mobility. Toho's new and improved FLX family of products measure intrinsic or thermal stress, expansion coefficients, and more. Advanced film thickness measurements of single/multi-layer films are performed with the Nanometrics' new NanoSpec II Systems and TohoSpec 3100.

Toyama Co., Ltd. 3816-1 Kishi, Yamakita-machi, Ashigarakami-gun Kanagawa, 258-0112, JAPAN Tel: +81-46-579-1411 https://www.toyama-en.com	Toyama designs and manufactures accelerator and synchrotron beamline component and systems. Toyama is fundamentally an engineering company, manufacturing ultra-precision systems for experimentation at the cutting edge of science. If you have a new concept that needs to be developed, then Toyama is the place to come. We have the technology and experience to turn your ideas into reality. In addition to our skills at developing new products, our long history of supplying scientific instrumentation means that we have produced a wide range of standard products. These standard items can meet the needs of many system requirements; alternatively they can be easily and quickly customised to meet your specific needs.
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Vacuum One 3717 N. Ravenswood – Suite 240 Chicago, IL 60613 Tel: 773-244-3102 https://www.vacuumone.com	Vacuum One is a manufacturers' representative firm in the Midwest. We represent the following companies.... □ Edwards Vacuum □ MDC Vacuum Products □ Insulator Seal Incorporated □ CTI-Cryogenics □ MKS Instruments/Granville-Phillips □ Polycold □ Gamma Vacuum □ KLA-Tencor □ Veeco □ Kaufman and Robinson, Inc. □ Advanced Energy □ Applied Thermal Control

WIENER Plein & Baus Corp.
202 N. Limestone Street
Suite 320
Springfield, OH 45503
Tel: 937-324-2420
https://www.wiener-us.com

WIENER Plein & Baus Corp. is providing a full line of electronics for detector read-out, data acquisition, experiment control and diagnostics.

Combining superior designed mechanic chassis with high quality, microprocessor controlled, low noise power supplies and a high level of integrated diagnostic and monitoring W-IE-NE-R became a world leader for powered chassis in all standards as VME/VME64x, VXI, PXI, ... In a joint venture between W-IE-NE-R and ISEG we provide the new high density, multi-channel low and high voltage power supply system MPOD / MMS which can house up to 480 independent high voltage, 80 low voltage channels or any mixture of low and high voltage. ISEG multi-channel modules offer highest stability and lowest ripple/noise and thus deliver cutting-edge solutions for high voltage applications. Adding a line of stand-alone HV power supplies ISEG is covering a range from 100V up to 100kV in different power classes.

In addition to our family of high performance controllers for VME and CAMAC with USB2 interface a new series of MESYTEC high resolution digitizers in VME as well as matching NIM front-end modules and a new VME display / bus-analyzer completes our line of instrumentation.

- WIENER: low voltage power supplies and systems, powered chassis [www.wiener-d.com]
- ISEG: High voltage power supplies, modules and multi-channel systems [www.iseg-hv.com]
- MESYTEC: analog and digital detector read-out electronics [www.mesytec.com]

X-Spectrum GmbH
Building 200/Innovation Village
Notkestr. 85
22607 Hamburg
Germany
Tel: +4915731711472
https://vlad@x-spectrum.de

Developed at CERN's laboratories, LAMBDA is based on the Medipix3 readout chip.

It is designed for synchrotron experiments requiring high spatial resolution, high sensitivity and extremely high speed.

LAMBDA is ideally suited for these applications:

- XPCS
- Time-resolved measurements
- Ptychography
- SAXS
- Diamond anvil cells and imaging.

Single-photon-counting circuitry means that LAMBDA provides effectively noise-free operation. This is critical for achieving high image quality during fast measurements and for discriminating against fluorescence.

LAMBDA's small pixel size (55 µm) means that it offers the best high-resolution imaging available, with flexible in-pixel circuitry.

XGLab Srl
Via Conte Rosso 23
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+39 02 4966 0460
https://www.xglab.it/

XGLab holds a leadership and innovative position in the field of radiation detectors and electronic instrumentation for X- and Gamma-ray spectroscopic analysis and imaging. XGLab is now part of Bruker Nano Analytics (BNA), a division of the Bruker Corporation, a global leader in scientific instruments and solutions for life sciences and materials research, as well as industrial process and quality control.

XIA LLC
31057 Genstar Road
Hayward, CA 94544
Tel: 510-401-5760
https://www.xia.com

XIA LLC invents, develops, and markets advanced digital data acquisition and processing systems for high rate x-ray spectroscopy at synchrotron facilities and other radiation detector applications in university research, national laboratories, and industry. Our core technology of high rate digital signal processing is applied to a diverse range of products from large multichannel systems, to benchtop units and compact low power processor cards for handheld instrumentation. Our product features include high rate elemental fast mapping, and data output rates in excess of 3 Mcps (FalconX). In addition to x-ray detector electronics, XIA offers a parallel product line of high speed digital signal processors for gamma detectors used for spectroscopy, timing and coincidence measurements. XIA is based in Hayward, California, on the east side of San Francisco Bay. Our multi-lingual staff currently supports product sales in over 30 countries on six continents.

GENERAL INFORMATION

Practical Matters

Locations

General sessions will be held in the Auditorium on the first floor of the APS conference center, Building 402. Vendor exhibits will be in the center's lower level and the atrium on the main level. Workshop locations are listed on the Comprehensive Program and posted at the registration desk.

Meals

The conference fee includes a continental breakfast and coffee breaks each day and the poster session reception. Buffet lunches will be served Monday through Wednesday in the tent outside of the Gallery on the lower level. If you pre-ordered lunches on your registration form, you will receive your tickets when you receive your meeting materials. (A limited number of extra lunch tickets are available for purchase at the registration desk.) Banquet tickets are nonrefundable. The Argonne cafeteria will be open for lunch; the Guest House restaurant it is open for dinner. The 401 Grill will be open for dinner throughout the meeting. A list of nearby restaurants is available at www.aps.anl.gov/About/Visiting/Restaurants.

Telephones and Messages

Messages for you can be left at the registration desk; the telephone numbers there are 630-252-9580 and 630-252-9581. The messages will be posted on a bulletin board by the entrance to the Auditorium. If you need to make a telephone call, a pay phone is located downstairs near the restrooms at the back of the Gallery, lower level. If you need to send or receive a fax, a fax machine is located in the APS User Office (Building 401, Rm. B1154). The number of this machine is 630-252-9250.

Transportation

Conference staff can make limousine reservations for you during the meeting as long as you make your request before 1:00 pm on Wednesday.

ATM

An automated teller machine is located in Building 233, behind the Argonne cafeteria. This machine accepts the following cards: American Express, Discover/Novus, The Exchange, Master Card, Plus, Visa, and 24 Access.

Computer Access

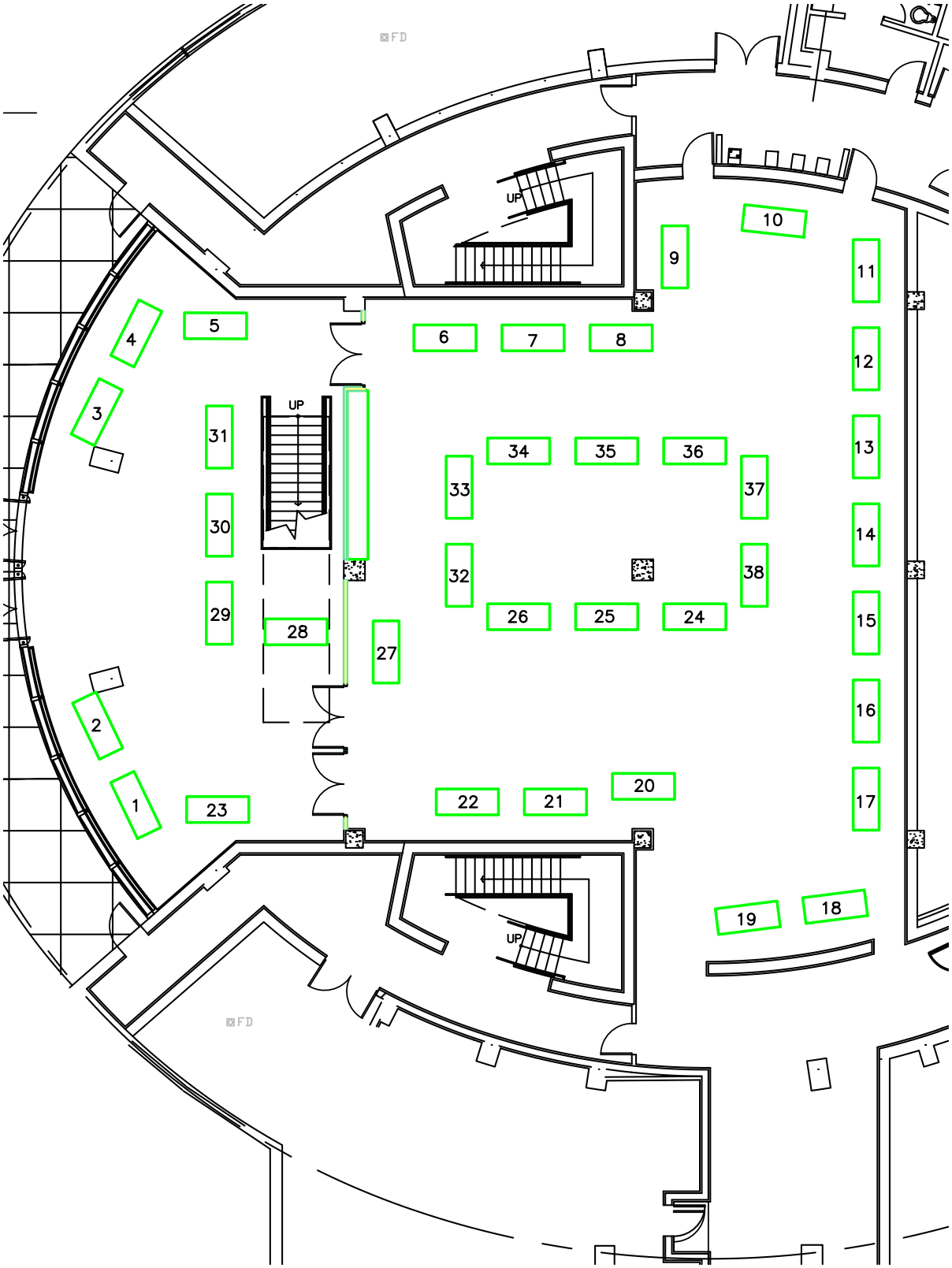
Public computer terminals are available in the Building 401 atrium behind the silver wall. Wireless access is also available in the Conference Center.

To use your laptop computer on the APS wireless networks, complete the following steps:

1. Open the wireless connection on your computer (either the 401 or 402 networks).
2. Read and accept the Argonne internet access policy, which will appear as a Web page on your desktop. After you click "accept," a registration Web page will appear.
3. The registration web page asks you for the following information:
    a. First and last name
    b. E-mail address
    c. Building and room where you will be located (use 402 conference center)
    d. Phone number where you can be reached on site (use 630-252-9090)
    e. Name of person you are visiting or conference you are attending
    f. Home institution
    g. Do you need to send e-mail directly to an off-site server?
    h. What is the duration of this registration? (You'll be given choices.)

If you have problems, please contact someone in the APS User Office (B1154, located immediately off the Conference Center atrium). Please do not share personal hotspots. This interferes with the Wi-fi network.

Exhibitor Location Map/Lower Gallery Level



Exhibitor Location Map/Lower Gallery Level

1 Teledyne Signal Processing Devices Sweden AB – GOLD SPONSOR

2 Leybold USA Inc. / Midwest Vacuum

3 USI Corporation

4 neaspec GmbH

5 HUBER Diffraktionstechnik

6 Agilent Technologies, Vacuum Products Division

7 Talend Inc.

8 Mahr Inc.

9 CINEL STRUMENTI SCIENTIFICI SRL

10 WIENER Plein & Baus Corp.

11 Applied Diamond, Inc.

12 Pfeiffer Vacuum

13 Nor-Cal Products

14 Alan Burrill Technical Sales

15 Starrett Tru-Stone Tech

16 Kurt J. Lesker Company

17 Bruker

18 Sydor Technologies

19 XIA LLC

20 Vacuum One

21 FMB Oxford

22 Spellman High Voltage Electronics Corporation

23 Rigaku Innovative Technologies, Inc.

24 Cosmotec, Inc.

25 Mirion Technologies (Canberra)

26 ABILITY ENGINEERING TECHNOLOGY INC

27 BellowsTech

28 RaySpec

29 Advanced Design Consulting USA, Inc.

30 attocube systems Inc.

31 XGLab Srl

32 MKS Instruments, Inc.

33 Newport Corporation

34 MPF Products Inc.

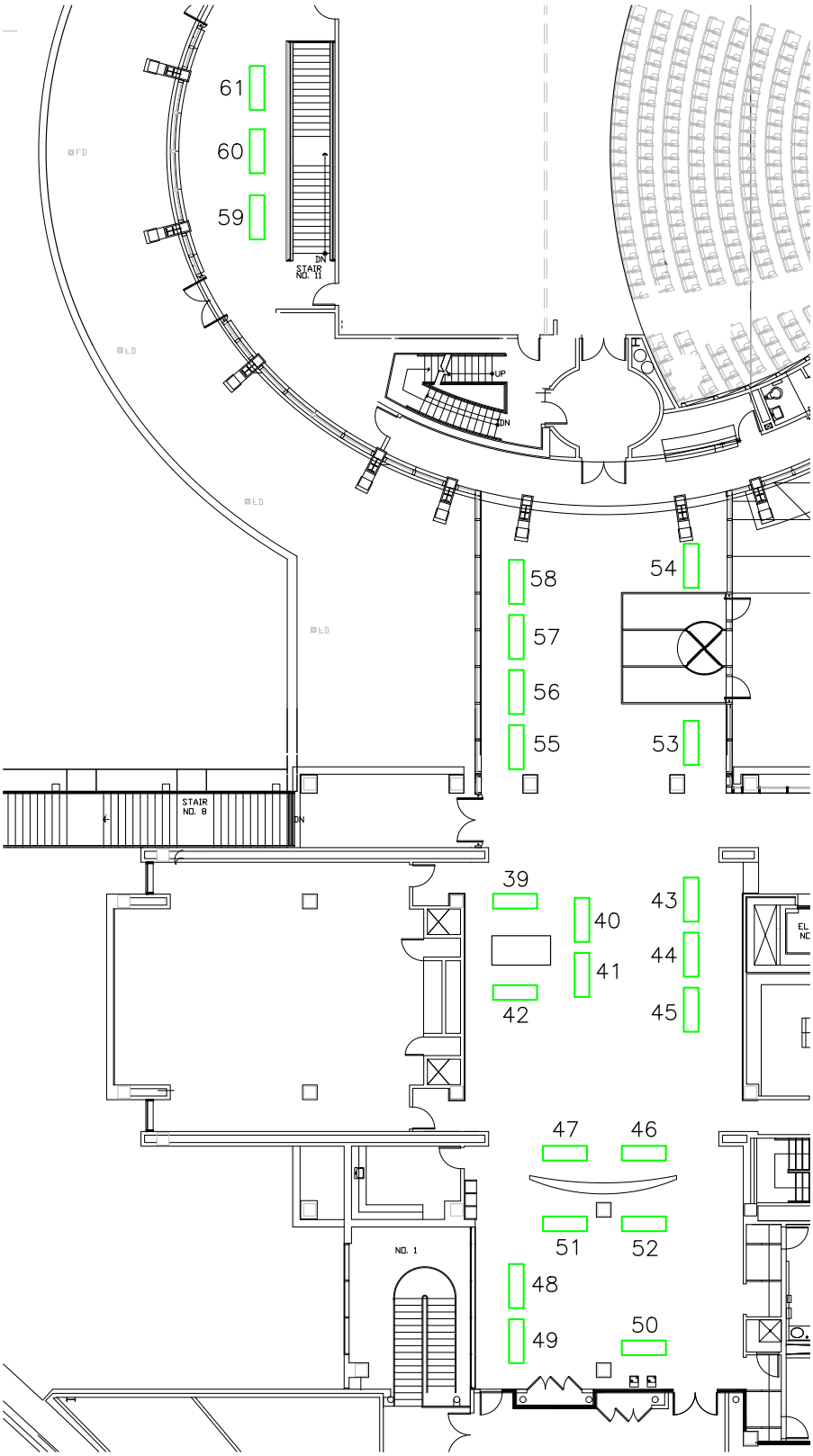
35 Aerotech Inc.

36 Anderson Dahlen - Applied Vacuum Division

37 Quantum Detectors

38 HIWIN

Exhibitor Location Map/Upper Atrium Level



Exhibitor Location Map/Upper Atrium Level

39 Rayonix, L.L.C.

40 AXILON

41 JTEC CORPORATION

42 IRELEC

43 VACOM Vakuum Komponenten & Messtechnik GmbH

44 SPECS-TII, Inc.

45 X-Spectrum GmbH

46 TDK-LAMBDA AMERICAS PROGRAMMABLE POWER DIVISION

47 Toyama Co., Ltd.

48 DECTRIS

49 Excillum Inc.

50 Toho Technology Inc.

51 OMS Motion, Inc.

52 Instrument Design Technology Ltd.

53 Argonne National Laboratory Electronics Fabrication Group

54 Meyer Tool & Manufacturing, Inc.

55 FREDERICKS COMPANY / TELEVAC

56 McCrone Group

57 KOHZU Precision Co. c/o Daniel F Crews, LLC

58 Princeton Instruments

59 Lion Precision

60 Andor Technology

61 Carl Zeiss X-ray Microscopy

ABOUT ARGONNE NATIONAL LABORATORY

- U.S. Department of Energy research facility
- Midwest's largest federally funded R&D facility
- Located in Lemont, IL, about 25 miles (40 km) southwest of Chicago, IL (USA)
- Conducts basic and applied research in dozens of fields
- 1,400 world-class staff scientists and engineers
- Unique suite of leading-edge and rare scientific user facilities

FOR MORE INFORMATION

please visit:

www.aps.anl.gov
www.anl.gov/cnm

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