Light Source Enabled Science
Room 319 - Session LS-MoM

Light Source Enabled ARPES

Moderators: Dr. Lucía Pérez Ramírez, CEA Saclay, **Dr. Nicholas Strange**, SLAC National Accelerator Laboratory

10:00am **LS-MoM-1 Depth-Resolved X-Ray Spectroscopy of Emergent Electronic and Magnetic States at Oxide Interfaces***, **Alexander Gray**,* Temple University **INVITED**

The emergence of novel electronic and magnetic states at correlated oxide interfaces is governed by a complex interplay of charge transfer, orbital reconstruction, and interfacial magnetism. In this talk, I will demonstrate how the combination of complementary synchrotron-based probes, including hard X-ray photoelectron spectroscopy (HAXPES), angle-resolved photoelectron spectroscopy (ARPES), polarization-dependent X-ray absorption spectroscopy (XAS), and resonant X-ray magnetic reflectivity, enables a comprehensive, depth-sensitive view of these phenomena in buried oxide heterostructures. Using $LaNiO_3/CaMnO_3$, $CaMnO_3/CaRuO_3$, $NdNiO_3/CaMnO_3$, and $VO_2/LaAlO_3/TiO_2$ interfaces as model systems, we reveal how interface engineering, defect chemistry, and interfacial charge transfer can stabilize emergent ferromagnetism and tune electronic phase transitions [1-3]. Looking forward, these synchrotron-enabled insights also establish a foundation for ultrafast studies at X-ray free-electron lasers (FEL), where intense IR or THz electric-field pulses can be used to manipulate interfacial electronic and magnetic states on their intrinsic timescales [4]. These studies highlight the unique power of combining multiple synchrotron techniques to disentangle coupled charge, spin, and orbital interactions at complex interfaces and provide pathways toward controllable oxide-based electronic and spintronic functionalities.

Author acknowledges support from the US Air Force Office of Scientific Research (AFOSR) under award number FA9550-23-1-0476; and from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Award No. DE-SC0024132.

[1] J. R. Paudel *et al.*, *Phys. Rev. B* **108**, 054441 (2023).
[3] D. Mondal *et al.*, *Nature Comm.* **14**, 6210 (2023).
[3] J. R. Paudel *et al.*, *Nano Letters***24**, 15195 (2024).
[4] A. M. Derrico *et al.*, *Adv. Mater.* **38**, e12328 (2026).

10:30am **LS-MoM-3 Layer-Specific Spin-Polarization in a Triple-Layer Ferromagnetic Oxide***, **Jonathan Denlinger**,* Lawrence Berkeley National Laboratory*; Prosper Ngabonziza,* Louisiana State University*; Alexei Fedorov,* Lawrence Berkeley National Laboratory*; Gang Cao,* University of Colorado Boulder*; James W. Allen,* University of Michigan, Ann Arbor*; G. Gebreyesus,* University of Ghana, Accra, Ghana*; Richard M. Martin,* Stanford University

The transport and magnetic properties of triple-layer oxides can be distinctly affected by the different structural environments of the outer versus central layers. Here we highlight the layer-specific *spin-polarized* electronic structure of the ferromagnetic triple-layer ruthenate $Sr_4Ru_3O_{10}$, using high resolution synchrotron angle- and spin-resolved photoemission spectroscopy (ARPES) [1]. Two separate narrow-band van Hove singularities (vHS) are found ∼30 meV below the Fermi-level at the zone center and at the zone-edge, which exhibit almost pure spin-polarization, but with opposite-sign. Comparison of the ARPES to spin-polarized DFT calculations quantifies the FM exchange splitting energy, and thus the predicted layer-specific spin polarization contributions to the magnetism, which is then indirectly evidenced by ARPES multi-zone matrix element intensities.

Furthermore, the vHS peaks exhibit dramatic Kondo-coherence-like temperature-dependence, that are the result of multi-orbital Hund metal physics. Fine T-dependent effects at various momenta, including oxygen-band spin-polarization and spin-dependent energy and momentum-shifts provide a more refined picture of the itinerant versus localized description of its magnetism. Finally, rotations of oxygen octahedra induce a zone-folded hybridization of opposite spin bands that break up the zone boundary vHS into smaller lower energy scale mini-vHSs that are relevant to the field-induced metamagnetism of the system.

[1] P. Ngabonziza et al. Phys. Rev. B **111**, 115146 (2025)

10:45am **LS-MoM-4 In-situ Strain Tuning of Electronic Order at a Light Source: Insights from μ-ARPES and μ-Diffraction***, **Yucheng Guo**,* Rice University*; Zhaoyu Liu,* Clemson University*; Na Hyun Jo,* University of Michigan, Ann Arbor*; Ji Seop Oh,* Sookmyung Women's University, Korea (Democratic People's Republic of)*; Yichen Zhang,* Rice University*; Aaron Bostwick, Chris Jozwiak, Nobumichi Tamura,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Makoto Hashimoto, Donghui Lu,* SLAC National Accelerator Laboratory*; Robert J. Birgeneau,* University of California, Berkeley*; Jiun-Haw Chu,* University of Washington*; Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Ming Yi,* Rice University

In quantum materials, the manipulation of atomic spacing and electron-cloud overlap enables precise control of the many-body Hamiltonian, influencing the material's ground state, excitations, phases, and competing orders. To investigate how these effects are manifested in the electronic band structure, we integrated a piezo-driven stress cell compatible with μ-ARPES and Laue μ-diffraction beamlines at the Advanced Light Source.

Using this capability, we investigate an intriguing phenomenon reported by P. Malinowski *et al.* [1], who demonstrated that continuously applied uniaxial strain can strongly suppress the superconducting transition temperature, Tc, in an optimally doped iron-based superconductor, while the underlying microscopic mechanism remains elusive.

In this presentation, we discuss in-situ uniaxial strain tuning of electronic correlations in an orbital- and momentum-resolved manner, using decoupled strain channels in $BaFe_2(As_{0.7}P_{0.3})_2$. Our results are largely consistent with a nematic quantum critical point scenario.

[1] P. Malinowski *et al.*, *Nature Physics* **16**, 1189–1193 (2020).

11:00am **LS-MoM-5 Large Exciton Binding Energy in a Bulk Van Der Waals Magnet from Quasi-1D Electronic Localization***, **Shane Smolenski**, Ming Wen, Qiuyang Li, Eoghan Downey, Adam Alfrey,* University of Michigan, Ann Arbor*; Wenhao Liu, Aswin Kondusamy,* University of Texas at Dallas*; Aaron Bostwick, Chris Jozwiak, Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Liuyan Zhao, Hui Deng,* University of Michigan, Ann Arbor*; Bing Lv,* University of Texas at Dallas*; Dominika Zgid, Emanuel Gull, Na Hyun Jo,* University of Michigan, Ann Arbor

Excitons, bound electron-hole pairs, influence the optical properties in strongly interacting solid-state systems and are typically most stable and pronounced in monolayer materials. Bulk systems with large exciton binding energies, on the other hand, are rare and the mechanisms driving their stability are still relatively unexplored. Here, we report an exceptionally large exciton binding energy in single crystals of the bulk van der Waals antiferromagnet CrSBr. Utilizing state-of-the-art synchrotron-based angle-resolved photoemission spectroscopy and self-consistent ab-initio *GW* calculations, we present direct spectroscopic evidence supporting electronic localization and weak dielectric screening as mechanisms contributing to the amplified exciton binding energy. Furthermore, we report that surface doping enables broad tunability of the band gap offering promise for engineering of the optical and electronic properties. Our results indicate that CrSBr is a promising material for the study of the role of anisotropy in strongly interacting bulk systems and for the development of exciton-based optoelectronics.

11:15am **LS-MoM-6 Probing Domain-Specific Charge Density Wave Dynamics and Strain Tunability in Bulk 1T-VTe2***, **Pratik Saud**,* Carnegie Mellon University, USA*; Sandy Adhitia Ekahana,* Carnegie Mellon University*; Aalok Tiwari,* Carnegie Mellon University, USA*; Mohan Bikram Neupane,* Purdue University, USA*; Sagnik Bajpeyi,* Carnegie Mellon University, USA*; Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Arnab Banerjee,* Purdue University, USA*; Simranjeet Singh, Jyoti Katoch,* Carnegie Mellon University, USA

In transition metal dichalcogenides, the emergence of a charge density wave (CDW) is highly sensitive to the material's dimensionality. While bulk and multi-layer 1T-VTe_2 host a robust CDW state, this ordered phase is unexpectedly suppressed in the monolayer limit. This contrast indicates that out-of-plane interactions are fundamental to stabilizing the CDW. Consequently, a rigorous, momentum-resolved investigation of the 3D bulk crystal is a requisite precursor to engineering these states in ultra-thin devices. Here, we utilize advanced synchrotron light sources to systematically investigate the structural and electronic phase transitions of pristine bulk 1T-VTe_2. We employ Laue microdiffraction (beamline 12.3.2) at the Advanced Light Source (ALS) to map local crystallographic symmetries, alongside high-resolution Angle-Resolved Photoemission Spectroscopy with micron-sized spatial resolution (microARPES) at the MAESTRO 7.0.2

beamline to track electronic dispersion. A key objective of this work is to spatially correlate these independent datasets to decouple lattice distortions from the CDW gap formation.

Temperature-dependent ARPES measurements reveal a dramatic phase evolution. At 500 K, the material exhibits a highly symmetric hexagonal Brillouin zone. Cooling to cryogenic temperatures triggers a macroscopic symmetry breaking, forming three distinct structural domains rotated 120 degrees relative to one another. Probing these individual domains enables the observation of highly directional, quasi-one-dimensional electronic features emerging from the symmetric parent state. Furthermore, this multi-domain landscape provides an opportunity to search for localized electronic states residing at the boundaries between these energetically equivalent regions. Next, we will present our work beyond static observation, where we introduce in-operando mechanical strain during photoemission measurements, to actively manipulate domain populations and tune their corresponding electronic signatures. By comprehensively detailing domain formation, boundary phenomena, and strain-engineered responses in the bulk, this research establishes a predictive framework for dimensional crossover effects. Ultimately, these insights lay the critical groundwork for future efforts to isolate, manipulate, and control fragile correlated phases within mechanically exfoliated two-dimensional heterostructures.

11:30am **LS-MoM-7 Observing the Electronic Response of a Mott Insulator at a Current-Induced Insulator-to-Metal Transition Using Transport-ARPES**, ***Cissy Suen***, Max Planck Institute for Solid State Research, University of Britsh Columbia, Germany*; Igor Markovic, Marta Zonno, Niclas Heinsdorf, Sergey Zhdanovich,* University of British Columbia, Canada*; Na Hyun Jo,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Michael Schmid,* Max Planck Institute for Solid State Research, Germany*; Philipp Hansmann,* Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany*; Steef Smit, Christine Au-Yeung,* University of British Columbia, Canada*; Valentin Zimmermann,* Max Planck Institute for Solid State Research, Germany*; Berend Zwartsenberg,* University of British Columbia, Canada*; Maximilian Krauloher,* Max Planck Institute for Solid State Research, Germany*; Sergey Gorovikov,* Canadian Light Source, Inc., Canada*; Chris Jozwiak, Aaron Bostwick,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Marcel Franz,* University of British Columbia, Canada*; Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Bernhard Keimer,* Max Planck Insitute for Solid State Research, Germany*; Andrea Damascelli,* University of British Columbia, Canada

The quasi-two-dimensional Mott insulator Ca2RuO4 exhibits a convergence of spin-orbit coupling and electronic correlations that lead to exciting quantum phenomena [1], including a rare insulator-to-metal transition (IMT) induced by a DC current [2]. While structural changes have been tracked by neutron diffraction [3], Raman scattering [4], and x-ray diffraction [5], the associated electronic changes had not been observed. Here we report angle-resolved photoemission spectroscopy (ARPES) results under DC current, which show a substantial reduction of the Mott gap, along with a change in the Ru t2g band dispersion [6]. We have also captured the high temperature Fermi surface, whose spectral features are unique from the current-induced metallic Fermi surface. In conjunction with a free energy analysis, our results demonstrate that the current-induced phase, albeit thermodynamically equivalent, is electronically distinct from the high-temperature zero-current metallic phase.

Combining ARPES with transport, i.e. transport-ARPES, has been rare given the complexity of disassociating real field- or current-driven physics from the effect of stray electric and magnetic fields on the outgoing photoelectron trajectory. By taking advantage of the micron-sized beam spot at the MAESTRO beamline (7.0.2) at the Advanced Light Source and careful core level spectrum analysis, we show that transport-ARPES can be extended to the study of any ARPES-suitable material. I will include an overview on transport-ARPES, as well as a brief outlook on the exciting prospects of in operando spectroscopy.

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[2] R. Okazaki et al., J. Phys. Soc. Jpn 82 (2013) 103702

[3] J. Bertinshaw et al., Phys. Rev. Lett 123 (2019) 137204

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[5] K. Jenni et al., Phys. Rev. Mat 4 (2020) 085001

[6] C.T. Suen et al., Nat. Phys. 20 (2024) 1757–1763

11:45am **LS-MoM-8 Investigation of Momentum Resolved Electronic Structure of Cr1.17Te2**, ***Sagnik Bajpeyi***, Carnegie Mellon University, USA*; Sandy Adhitia Ekahana,* Carnegie Mellon University*; Aalok Tiwari,* Carnegie Mellon University, USA*; Mohan Bikram Neupane,* Purdue University, USA*; Pratik Singh Saud,* Carnegie Mellon University, USA*; Chris Jozwiak, Eli Rotenberg, Aaron Bostwick,* Lawrence Berkeley National Laboratory, US*; Arnab Banerjee,* Purdue University, USA*; Simranjeet Singh, Jyoti Katoch,* Carnegie Mellon University, USA

Chromium tellurides have attracted significant interest due to the strong interplay between electronic correlations and crystal structure. Among them, Cr1.17Te2 is a transition-metal chalcogenide that exhibits complex electronic behavior arising from non-stoichiometry and strong Cr–Te hybridization. Here, we investigate the electronic structure of Cr1.17Te2 using high-spatial-resolution angle-resolved photoemission spectroscopy (microARPES) performed at the MAESTRO Beamline of the Advanced Light Source.

We will present momentum-resolved band dispersion measurements acquired at 10 K using 84 eV photons with varying light polarizations, together with core-level spectroscopy of Cr and Te orbitals and out-of-plane kz dispersion measurements. Potassium surface dosing was further employed to tune the chemical potential and investigate the evolution of electronic states near the Fermi level. Our photon-energy-dependent measurements reveal a periodicity that deviates from expectations based on X-ray diffraction data, suggesting a more complex three-dimensional electronic structure than previously anticipated. These results motivate future soft X-ray ARPES measurements in the 300–700 eV range to further elucidate the intrinsic bulk electronic structure of Cr1.17Te2 and resolve the origin of this discrepancy.

Light Source Enabled Science
Room 319 - Session LS-MoA

Light Source Enabled Science

Moderators: Prof. Alexander Gray, Temple University, **Prof. Juanita Hidalgo**, NYU

1:30pm **LS-MoA-1 Advancing the Sample Space to Elevate the Power of Resonant X-ray Scattering*, Philip Ryan,*** Argonne National Laboratory, USA **INVITED**

Deploying *in-situ* strain withelectrical *multi-modal* x-ray scattering measurements has allowed for powerful experimental configurations deepening our understanding of complex quantum phenomena. Touching upon a few recent topics e.g., nematic behavior in Fe superconductors (1-4) and quantum paraelectric behavior in $SrTO_3$ membranes (5) I'll demonstrate the value-added power of investing in the sample space and overview our plans to explore dopant-vacancy color center qubit behavior with symmetry and strain combining photoluminescent spectroscopy and x-ray scattering.

The ability to measure and control structure, symmetry or domain population of a twinned system, like an orthorhombic crystal or magnetic orientated domains can be a critical sample control parameter to study intricate quantum behaviors. In the iron-based superconductor, electronic nematicity is coupled to both the lattice and the conducting electrons leading to both structural and transport measurements sensitive to nematic fluctuations. While spin driven nematicity is prevalent in Fe pnictides, the role of spin versus orbit in the chalcogenide nematic behavior has been under investigation. The consortium of electrical and x-ray scattering measurements keenly addresses the relationship of lattice, spin and orbital order in the nematic phase space. $SrTO_3$ is a ubiquitous prototype material but is itself an intriguing enigmatic host of quantum behaviors, using strain as a tuning parameter we investigate the transition from classical to quantum behaviors and consider the unbounded potential studies deploying this combination of strained single crystal membranes with resonant x-ray scattering.

1.Strain-Switchable Field-Induced Superconductivity, Joshua J. Sanchez [https://arxiv.org/search/cond-mat?searchtype=author&query=Sanchez%2C+J+J], et al., Science Advances 9, eadj5200(2023). DOI:10.1126/sciadv.adj5200 [https://doi.org/10.1126/sciadv.adj5200] 2.Suppression of superconductivity by anisotropic strain near a nematic quantum critical point, P. Malinowski, et al., Nature Physics, 1-5, (2020)3.Spontaneous orbital polarization in the nematic phase of FeSe. Connor A. Occhialini, et al., Nature Materials 22, 985 (2023). doi:10.1038/s41563-023-01585-2 4. The transport–structural correspondence across the nematic phase transition probed by elasto X-ray diffraction. J.J. Sanchez, Nat. Mater. (2021) 5.Li J., et al. The classical-to-quantum crossover in the strain-induced ferroelectric transition in SrTiO3 membranes. Nat Commun 16, 4445 (2025

2:00pm **LS-MoA-3 Monolithic 2D Multilayer Laue Lens Optics for Hard X-ray Nanoimaging*, Wei Xu,*** *Zirui Gao, Weihe Xu, Nathalie Bouet, Juan Zhou, Hanfei Yan, Xiaojing Huang, Ming Lu, Mingyuan Ge, Yong Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) are promising X-ray optics for nanometer-scale, high-efficiency focusing in the hard X-ray regime. Achieving high-performance two-dimensional (2D) focusing requires precise angular and translational alignment of two sets of linear MLLs, involving eight degrees of freedom of motion. For nanoimaging with sub-10 nm resolution, the tolerance for the relative angular alignment between the lenses is approximately 0.01°. Such stringent requirements pose significant challenges for microscopy systems and have hindered the application of MLLs in synchrotron light sources. In this work, we present the development of an advanced generation of monolithic 2DMLLs that address these challenges through a microfabrication-enabled assembly approach.

The monolithic optics were assembled using a silicon-based micro-electro-mechanical systems (MEMS) template. The template incorporates microfabricated alignment and holding structures that enable precise control of the angular and lateral positions of the MLLs mounted on the template. By engineering the alignment microstructures, an angular alignment resolution on the order of a few millidegrees was achieved, which was characterized by white-light interferometry and validated by synchrotron X-ray measurements.

The performance of the monolithic 2D MLLs was demonstrated at the Hard X-ray Nanoprobe (HXN) beamline at NSLS-II using ptychographic imaging. High-resolution 2D imaging achieved sub-10 nm spatial resolution, as verified by Siemens star test patterns. Furthermore, the optics were used to perform nanoscale X-ray tomography, revealing internal interfacial grain boundary structures in a $CoFe_2O_4$-$Ce_{0.8}Gd_{0.2}O_2$-based mixed ionic-electronic conductors (MIECs) system with nanoscale resolution.

This work demonstrates an effective and robust approach to simplifying alignment while advancing the performance of 2D MLL optics. The new optics with high alignment accuracy represent an important step toward the development of monolithic 2D MLL optics for hard X-ray nanoimaging.

2:15pm **LS-MoA-4 Development of Advanced High-Speed Fly-Scan Technology for sub-10 nm Hard X-Ray Imaging at NSLS-II*, Weihe Xu,*** *Takenori Shimamura,* Brookhaven National Laboratory*; Dmitri Gavrilov,* brookhaven National Laboratory*; Huijuan Xu,* Brookhaven National Laboratory*; Wei Xu, Hanfei Yan,* brookhaven National Laboratory*; Nathalie Bouet, Juan Zhou, Randy Smith, Jun Ma, Xiaojing Huang, Yong S. Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) offer significant advantages over traditional diffractive focusing optics, such as zone plates (ZPs), particularly in terms of efficiency when focusing hard X-rays to 10 nm and below. The resulting increase in photon flux density drives the need for faster fly-scan capabilities to minimize radiation damage and improve data acquisition rates.

To answer this challenge, we developed a next-generation scanning X-ray microscopy testbed designed for high-speed data acquisition. The system demonstrated sub 10-nm ptychographic imaging, and achieved data acquisition rates exceeding 1 kPPS (kilo-points-per-second) while being fully compatibility with the Experimental Physics and Industrial Control System (EPICS) environment used at NSLS-II.

This system, called RASMI (RApid Scanning Microscopy Instrument) [1], is a stand–alone microscope that uses a modular design to accommodate either two orthogonally arranged 1D multilayer Laue lenses (MLLs) or a single 2D optic—such as a zone plate or a monolithically assembled 2D MLL—for point focusing. RASMI supports both sample–scanning and 2D–optics–scanning modes of operation through the use of interchangeable modules. In the sample–scanning mode, the sample is moved during imaging experiments while the focusing optics remain stationary. This approach is insensitive to the structural variations in the incoming X–ray wavefront, ensuring consistent illumination across the entire sample. In the 2D–optics–scanning mode, the 2D optic is moved while the sample remains stationary. This approach can achieve higher scanning speeds, particularly when working with heavy or bulky samples, such as large environmental or in-situ/in-operando experimental cells. Both scanning modes use a laser interferometer as the fast-axis encoder for position data acquisition. The entire RASMI control system is EPICS compatible. The developed microscope can be operated in both time- or position-triggering modes with the maximum photon flux- and detector-limited rate of 1.25 kPPS. The 2D X-ray image results show ~6 nm resolution at sample scanning and ~8 nm resolutions at 2D optics scanning [2]. The developed fly–scan technology has already been implemented in the user instrument at the Hard X–ray Nanoprobe (HXN) beamline at NSLS–II. In this presentation, we also highlight preliminary work aimed at further increasing position–triggered data acquisition speeds.

REFERENCE:

1. Weihe Xu, et al., *Rev. Sci. Instrum.* 95, 113705, Nov 2024
2. Weihe Xu, et al., *Optics Continuum*, 5, 3 937-943, Mar 2026

2:30pm **LS-MoA-5 A Beamline for Probing Morphology and Dynamics of Thin Film Materials at the Advanced Photon Source*, Joseph Strzalka,*** Argonne National Laboratory

Feature beamline 9-ID at the recently upgraded Advanced Photon Source hosts the program in nanoscale structure, kinetics and dynamics, focusing on surfaces and interfaces of soft materials. The beamline is tunable over the range 6-25 keV, with highly coherent x-rays provided by a revolver undulator with a double crystal monochromator. Two transfocators focus the beam to about a 5 um spot size at the sample. A robust diffractometer allows for alignment of thin film samples in a variety of sample environments for operando studies in a horizontal grazing-incidence geometry. An in-air area detector captures wide-angle scattering (GIWAXS) while a large vacuum flight path with an in-vacuum pixel array detector accommodates sample-detector distances from 3- 20 m for GISAXS and also grazing-incidence x-ray photon correlation spectroscopy (GI-XPCS) probing

dynamics over time scales from 10^{-3} to 10^{3} s. Early experiments at 9-ID make use of these capabilities to study the structure and dynamics of organic mixed ionic electronic conducting materials, organic semiconductors, block copolymers for separation science and perovskite-based materials for energy applications.

Acknowledgments: This work would not be possible without contributions from the 9-ID CSSI beamline development team: Ray Ziegler, Jayson Anton, Sunil Chitra, Miaoqi Chu, Peco Myint,Jonathan Knopp, Luca Rebuffi, Xianbo Shi, Deming Shu, Sunil Bean, Ashish Tripathi, Chasen Wolford, Luis Diaz, Steven Kearney, Kevin Wakefield, Altaf Khan, Dana Capatina, Miaoqi Chu, Peco Myint, Hannah Parraga, Scientific Co-Leads Zhang Jiang and Jin Wang, and Dynamics and Structure group leader Suresh Narayanan and team member Hongrui He. We are grateful for collaborations with the groups of Prof. Jonathan Rivnay (Northwestern University) and Prof. Alamgir Karim (University of Houston), Prof. Po-Chun Hsu (University of Chicago) and Prof. Wanyi Nie and Prof. Hsinhan Tsai (SUNY Buffalo). This research was performed on APS beam time award(s) (DOI: https://doi.org/10.46936/APS-189194/60013707, https://doi.org/10.46936/APS-190153/60014220 , https://doi.org/10.46936/APS-190281/60014340 , https://doi.org/10.46936/APS-191475/60015201) from the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility at Argonne National Laboratory, and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

2:45pm **LS-MoA-6 The Role of Artificial Intelligence and Spectral Databases in Minimizing Analysis Errors, Illustrated with EXAFS, XES, and Core Level Photoemission***, **Jeff Terry,*** Illinois Institute of Technology

We have developed artificial intelligence-based methodologies that can be used to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS), X-ray Emission Spectroscopy (XES), and core level X-ray Photoelectron Spectroscopy (XPS). These efforts address persistent reproducibility problems that slow research progress and inhibit effective technology transfer and manufacturing innovation in materials science and related disciplines.

Our initial work focused on the analysis of EXAFS spectra collected at synchrotron radiation facilities. A machine learning approach, based on a genetic algorithm, was developed to fit measured spectra and extract relevant structural parameters. In the current approach, a set of possible chemical compounds, represented by feff.inp input files, that may be present in the sample. The algorithm then identifies the structural scattering paths from these candidate compounds that best reproduce the experimental measurement. The automated analysis searches for the primary EXAFS path contributors, calculates a goodness-of-fit value, and uses that metric to help identify the chemical moieties present in the material.

The resulting analysis package, EXAFS Neo, is an open-source Python code that uses Larch and FEFF to calculate and fit EXAFS paths. More recently, we have expanded this artificial intelligence framework beyond EXAFS to include XES and XPS analysis. These extensions make use of curated spectral databases for X-ray emission and core level photoemission, providing reference data that can be compared systematically with experimental spectra. By combining machine learning methods with database-driven spectral comparison, the analysis can reduce operator bias, improve consistency across users and laboratories, and provide more reproducible identification of chemical states, local bonding environments, and electronic structure signatures.

Together, these developments demonstrate how artificial intelligence, physics-based modeling, and experimentally grounded spectral databases can be integrated to minimize analysis errors in X-ray spectroscopies. The EXAFS Neo package and related information are available at: https://plutonium.phys.iit.edu/~jeff_terry/exafsneo.html or by contacting the speaker.

3:00pm **LS-MoA-7 Reliable Quantification of Oxygen Vacancies in Ferroelectric Hafnia Using Synchrotron-Based X-Ray Photoelectron Spectroscopy***, **Lucía Pérez Ramírez,*** *Tom Iung, Vineeta Yadav, Christophe Lubin,* CEA Saclay, France*; Uwe Schroeder, Florian Wunderwald,* Namlab, Germany*; Luis Azevedo Antunes, Alfred Kersch,* Munich University of Applied Sciences, Germany*; Tyson C. Back,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Conan Weiland,* NIST*; Mickael Gros-Jean,* ST Microelectronics, France*; Nicholas Barrett,* CEA Saclay, France **INVITED**

Oxygen vacancy (V_O) is the most common anion defect observed in metal oxides. Its presence can effectively alter the electronic and physico-chemical properties of oxides thin films, thus determining the overall performances of entire devices built on these materials. This is the case of ultra-thin ferroelectric hafnium oxide (HfO_2) films used for emergent non-volatile memory and logic devices. As it has been demonstrated that V_O have a significant impact on the stabilization of the polar orthorhombic phase, responsible for hafnia's ferroelectric character [1,2], determining their global concentration in hafnia layers is crucial for optimal device engineering. Moreover, their migration during electrical field cycling can modify the internal field of the device, affecting the coercive voltage (E_C) and remnant polarization (P_R) values [3]. It is thus of major importance to have an insight on the V_O distribution profile along the hafnia ferroelectric film.

So far, X-ray photoelectron spectroscopy (XPS) combined with Ar^+ ion sputtering has been the preferred method for V_O quantification and depth-profiling, but this is an ill-chosen approach given its destructive character. Here, we show that the use of non-destructive, hard X-ray photoemission (HAXPES) using synchrotron radiation ought to be favored [4], in order to avoid the artifacts introduced by the sputtering process. The particular example of V_O quantification in hafnia appears as a good occasion to review the basics of core-level spectral analysis, focusing on the Hf 4*f* doublet, as widespread mistakes in literature with wrong fitting procedures unfortunately hinder the reliability of quantitative analysis. Finally, we disprove the erroneous assignation of one of the O 1s core-level peak components to the presence of V_O. We demonstrate that there is no concrete evidence to support the theory that associates this component to a charge transfer to second nearest neighbor oxygen anions upon a V_O creation. It is more judicious to assign the O 1s high-binding energy components to physisorbed or chemisorbed species. Our conclusions are supported by careful comparison between XPS/HAXPES experimental results and first-principles calculations [5]. We provide clear indications for reliable analysis and interpretation of the photoemission data, which should allow progress in materials engineering of ferroelectric devices.

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3:30pm **LS-MoA-9 A Proposal for Fully Coherent nanoARPES: Probing Electronic Phase at the 10 nm Scale***, **Aaron Bostwick,*** *Chris Jozwiak, Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Simon Moser,* Ruhr-University Bochum, Germany

Current nanofocused ARPES experiments have achieved ~100 nm spatial resolution, bringing the power of ARPES to microscopic samples and device geometries. Here we propose a new experiment— "Fully Coherent ARPES" — targeting spatial resolutions of 10 nm, where fundamentally new physics becomes accessible. At this length scale, true low-dimensional systems become directly accessible, including 1D edge states, quantum Hall states, and isolated nanotubes, as well as potentially 0D quantum dots and materials with nanoscale electronic phase segregation such as high-Tc_cc superconductors.

Achieving this resolution requires a move to higher photon energies (~200 eV) and a transmission rather than reflection geometry, with the increased coherent flux of the 4th generation synchrotrons offsetting reduced cross sections. When the beam spot approaches or falls below the electron coherence length, the photoemission process enters a fully coherent regime. In analogy with Fourier ptychography, interference effects can then be exploited to extract electronic phase variations induced by defects, strain, and structural inhomogeneities at sub-beam-size length scales — a capability with no current equivalent in electronic structure measurements.

4:00pm **LS-MoA-11 Probing Magnetic Interactions with Coherent Soft X-ray Scattering**, ***Andi Barbour,*** Brookhaven National Laboratory **INVITED**

The Coherent Soft X-ray (CSX) beamline at the National Synchrotron Light Source II (NSLS-II) welcomed its first facility users just over a decade ago, providing world–leading coherent X-ray flux in the soft X-ray regime. This capability has enabled fresh perspectives on a wide range of materials and has driven new insights, including the development and application of computational techniques that accelerate discovery—for example, deep-learning denoising models for X-ray Photon Correlation Spectroscopy (XPCS) data and Coherent Correlation Imaging (CCI). In this talk, I will highlight impactful results, along with the computational methods behind them, that reveal the spatiotemporal dynamics of magnetic systems, ranging from domain-wall motion to coherent rotational control of skyrmion lattices.

4:30pm **LS-MoA-13 Alloy Oxidation for Corrosion Mitigation: Synchrotron Based X-Ray-Photoemission Electron Microscope (XPEEM) Studies from NiCr to High Entropy Alloys**, *Keithen Orson,* University of Virginia*; Jurek Sadowski,* Brookhaven National Laboratory*; Yuran Niu, Alexei Zakharov,* Max IV Laboratory, Sweden*;* ***Petra Reinke,*** University of Virginia

Oxide layers are critical to protect alloys but design prioritizes bulk properties which leads to a narrow compositional and microstructural range to optimize environmental resilience. We study the initial reaction steps during the transformation of alloy to oxide in a kinetically limited regime (T < 800 ° C). We used XPEEM in the study of oxidation for binary (NiCr), ternary (NiCr with Mo or W), and septenary dual phase compositionally complex alloys (CCA).

XPEEM captures chemical, structural, and temporal evolution of the oxide for several grains or phases at the same time. The multi-mode capabilities access work functions, surface structure (m-LEED), and chemistry via XAS/ XPS and nanoscale resolution. The video rate time resolution allows operando studies with chemical sensitivity. The XPEEM studies are combined with (i) laboratory XPS, (ii) synchrotron based ambient pressure XPS, and, in the future, (iii) ToF-SIMS to access sub-surface alloy composition.

We will show oxidation as a function of crystallographic orientation for NiCr, and discuss the role of Mo/ W in moving the oxidation reactions to a preference for chromia over NiO. Several surface orientations were observed simultaneously and confirmed with EBSD analysis. The distribution of chromia islands was extracted from single-energy, time resolved images (operando mode) and hyperspectral XAS images. The analysis of the image stacks required alignments, distortion and brightness correction, linear combination analysis and cosine similarity to yield the composition Cr/Cr_2O_3 for each pixel as a function of oxidation time. The corresponding workflow and code are published. Significant differences are observed as a function of surface orientation but the endpoint for chromia island growth is controlled by Cr supply from the alloy (Figure 1). In contrast, for the ternary alloy (NiCr with Mo/W) the initial adsorption kinetics differ with orientation but chromia always grows in a layer-by-layer mode along [0001]. An atomic scale mechanism which favors specific O-adsorption sites contributes to this development.

For the two-phase septenary alloy $Al_{0.3}Cr_{0.5}Fe_2Mn_{0.25}Mo_{0.15}Ni_{1.5}Ti_{0.3}$ (Figure 2) we are interested in the speciation of elements in the two phases FCC and $L2_1$, their oxides, and the sharpness of the interface. We focus on hyperspectral XAS images for 6 out of the 7 elements for native oxide, clean and oxidized alloy. The alloy design achieved identical work function for both phases but the sharp interface at the boundary remains a breaking point. We will compare the element speciation between the phases in alloy and oxide and discuss the challenges of oxide identification with XAS.

4:45pm **LS-MoA-14 Bragg-Enhanced XAS for Monitoring Real-Time Reactions at Interfaces**, ***Karthika Madathil,*** Lawrence Berkeley National Laboratory (LBNL)*; Alisson Thill,* Universidade Federal do Rio Grande do Sul, Brazil*; Cheng Wang,* Lawrence Berkeley National Laboratory (LBNL)*; Baran Eren,* Weizmann Institute of Science, Israel*; Slavomir Nemsak,* Lawrence Berkeley National Laboratory (LBNL)

Heterogeneous catalysis is central to addressing global energy and environmental challenges. Detailed understanding of Interfacial phenomena during catalysis is limited via traditional X-ray absorption spectroscopy (XAS) due to low temporal resolution arising from the small volume of the interfacial region and the low signal to noise ratio. With Bragg-enhanced XAS (BEXAS) we incorporate diffraction optics into the material of interest using customized periodic nanopattern design enabling coherent addition of scattered intensity. Combining the element specific sensitivity of soft x-rays and intensity amplification from constructive scattering, we capture transient signals arising from chemical changes at thin interfaces. In this work we demonstrate BEXAS for monitoring real time interfacial dynamics in model cerium oxide samples. The evolution of XAS was monitored during heating and gas phase annealing of the sample. The experimental scattering data is compared with simulation results to connect the observed changes in scattered intensity to changes in interfacial chemical composition and structure during the reactions. BEXAS allows the expansion of XAS to the time domain, which is critical for understanding interfacial reactions and investigating transient states which are crucial for developing new catalysts.

5:00pm **LS-MoA-15 Novel Lattice-Matched Substrates for Scalable III-N Power Electronics**, ***Amitayush Jha Thakur,*** Argonne National Laboratory, India

Next-generation power conversion technologies will be central to a highly electrified energy system, motivating new materials and manufacturing approaches for power electronics built for speed, scale, and resilience. This work focuses on crystalline, electrically conductive substrates for III-nitride power electronics and the co-design of commensurate heterostructure interfaces for AlGaN growth. Lattice-matched substrates such as ScB_2 and $Ta_{1-x}Hf_xC$/TaC offer new opportunities for AlGaN heteroepitaxy by reducing interfacial strain while providing higher thermal and electrical conductivity than conventional substrates such as Al_2O_3 or SiC. ScB_2 is lattice matched to approximately $Al_{0.6}Ga_{0.4}N$, while $Ta_{1-x}Hf_xC$/TaC provides tunable lattice matching around $Al_{0.5}Ga_{0.5}N$. Preliminary X-ray characterization, including XRD, XPS, and XAS, probes crystallinity, orientation, chemical composition, charge state, and local electronic structure across multiple length scales, establishing an initial foundation for understanding structure–function relationships in novel AlGaN/substrate interfaces.

5:15pm **LS-MoA-16 Studying Energy Materials with Bragg Coherent Diffractive Imaging**, ***Luxi Li,*** Argonne National Laboratory

Coherent X-ray diffraction methods provide unique opportunities to probe nanoscale structural heterogeneity in energy materials. With the recent upgrade of the Advanced Photon Source, the coherent X-ray flux has increased by up to two orders of magnitude, significantly expanding the capabilities of coherence-based imaging techniques. Among these methods, Bragg coherent diffractive imaging (BCDI) enables three-dimensional imaging of morphology, crystal structure, and internal strain fields in individual crystalline grains without the need for imaging optics.

In this presentation, I will highlight recent applications of BCDI to energy storage and conversion materials, with emphasis on how nanoscale strain, defect evolution, and morphological changes can be directly visualized under relevant conditions. These measurements provide insight into how local structural evolution influences materials performance, degradation, and functionality. I will also discuss how the upgraded APS enables new opportunities for operando and statistically meaningful BCDI studies, including faster measurements, improved sensitivity to weakly scattering systems, and the possibility of tracking dynamic structural processes in complex energy materials.

Light Source Enabled Science
Room 319 - Session LS-TuM

Light Source Enabled Energy Science

Moderators: Dr. Andi Barbour, Brookhaven National Laboratory, **Dr. Philip Ryan**, Argonne National Laboratory, USA

8:00am **LS-TuM-1 Surface Sensitive and In-Situ Characterization of Perovskite Materials for Energy Conversion***, Juanita Hidalgo,* New York University **INVITED**

Developing new energy conversion technologies is a critical scientific challenge to address global energy demand and global warming. Perovskite-type materials are particularly important because they exhibit electronic and or ionic conductivity, enabling a wide range of energy-related applications, including photovoltaics, fuel cells, and electrolysis cells. Lead halide perovskites (APbX3) have emerged as promising absorber layers for low-cost solar cells, while perovskite oxides (ABO3) are widely used as electrodes and catalysts in solid-state electrochemical systems. However, the perovskite crystal structure can be unstable and undergo phase transformations under external stressors. To investigate the surface structural and chemical properties of these materials, my work employs advanced synchrotron-based in-situ characterization techniques, including grazing-incidence wide-angle and small-angle x-ray scattering (GIWAXS/GISAXS) and near-ambient-pressure X-ray photoelectron spectroscopy (NAP-XPS). First, my talk will address the instability of lead halide perovskites under exposure to humidity and air, and the complex relationship between structure, properties, and performance in solar cell applications. Using in-situ GIWAXS, we investigated the undesired phase transformations that occur under humid air and humid nitrogen environments, revealing a synergistic effect between water and oxygen that accelerates degradation. Second, I will discuss the high-temperature reduction of perovskite oxides, which leads to the formation of embedded metal nickel nanoparticles through a process known as exsolution. These nickel nanoparticles can act as catalysts for electrochemical reactions relevant to energy conversion and storage. Using simultaneous in-situ XPS and GISAXS, we tracked nanoparticle formation through the reduction of nickel oxide to the metallic state and the corresponding structural evolution observed by GISAXS. Therefore, understanding the mechanisms governing perovskite phase transformations and establishing correlations between structure, chemistry, and properties is essential for tuning and optimizing these materials to achieve more robust, stable, and efficient energy technologies for real-world applications.

8:30am **LS-TuM-3 Energy Science Research Using In Situ and Operando Soft X-ray Spectroscopy at the National Synchrotron Light Source II: Science Highlights and Future Plans***, Iradwikanari Waluyo,* Brookhaven National Laboratory

From catalysts and fuel cells to batteries and corrosion-resistant superalloys, the In situ and Operando Soft X-ray spectroscopy (IOS, 23-ID-2) beamline at the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL) provides versatile experimental techniques to enable impactful science. The IOS beamline provides capabilities for ambient pressure X-ray photoelectron spectroscopy and X-ray absorption spectroscopy for revealing the dynamic evolution of the chemical and electronic states of energy materials under realistic working conditions. I will present recent research highlights, including (1) characterizing the surface chemical state of single-atom alloy model catalysts under oxidizing and reducing conditions, (2) understanding the reaction mechanism of industrially relevant heterogeneous catalytic reactions such as CO_2 hydrogenation, CH_4 conversion, and ethylene epoxidation, and (3) optimizing novel materials synthesis through tunable metal exsolution from perovskites. I will also give an overview of ongoing short term and long term upgrades with the aim to enable multi-modal ambient pressure soft X-ray spectroscopy at IOS, which will allow researchers to obtain comprehensive electronic and chemical information for energy materials in operating conditions at relevant time scales.

8:45am **LS-TuM-4 Operando Soft X-Ray Spectroscopy of Electrochemical Interfaces: From Reaction Cell and Sample Design to Mechanistic Insight***, Santosh Kumar,* Diamond Light Source Ltd., UK*; James J. C. Counter,* University of Manchester, UK*; David C. Grinter, Matthijs A. van Spronsen, Pilar Ferrer,* Diamond Light Source, UK*; Christopher M. Zalitis, Tugce Eralp Erden,* Johnson Matthey Technology Centre, UK*; Roger A. Bennett,* University of Reading, UK*;* ***Georg Held,*** Diamond Light Source, UK

Synchrotron-based *operando* soft X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) enable element-specific probing of electrochemical interfaces under realistic conditions but require advanced reaction cell and sample designs to bridge aqueous electrochemistry and vacuum-based detection. We present a modular spectro-electrochemical flow cell and window-free working electrode assembly (WEA) compatible with near-ambient-pressure XPS and NEXAFS. The platform combines interchangeable SiN_x or polymer membranes (such as Nafion™) with controlled hydration, enabling stable in-situ measurements under electrochemical operation. Using CuO_x- and IrO_x-based electrodes, we demonstrate tracking of redox processes, surface hydration, and oxygen evolution chemistry. *Operando* XPS and NEXAFS reveal potential-dependent metal oxidation and the formation of reactive oxygen species, providing direct insight into reaction mechanisms at electrochemical interfaces. This approach establishes a versatile methodology for soft X-ray studies of electrocatalysts.

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1. *Catalyst-Coated Mesoporous Carbon–Membrane Electrode Assembly for In-situ Soft X-ray XPS and NEXAFS Studies of Electrocatalytic Interfaces*, **ACS Electrochemistry** (2026) DOI: 10.1021/acselectrochem.5c00554.

2. *An Electrochemical Flow Cell for Operando XPS and NEXAFS Investigation of Solid–Liquid Interfaces*, **J. Phys. Energy** 6,036001 (2024). DOI: 10.1002/cctc.202400937

9:00am **LS-TuM-5 Substrate-Mediated Doping Reshaping Interfacial Energetics in Organic Electronics***, Xiane Li, Slavomir Nemsak,* Advanced Light Source, Lawrence Berkeley National Laboratory

Energy level alignment (ELA) at electrode/organic-semiconductor interfaces governs charge generation, transport, and injection in organic electronic and energy-conversion devices. However, ELA is typically characterized under ultra-high vacuum, whereas practical devices operate in ambient environments where water is ubiquitous. The influence of water on interfacial energetics therefore remains largely unresolved. Here we probe the evolution of ELA in the presence of water using operando ambient-pressure X-ray photoelectron spectroscopy combined with Kelvin probe measurements. We find that water molecules strongly reshape the interfacial electronic structure by screening the spontaneous charge transfer that forms interface dipoles under vacuum. This screening suppresses dipole formation at interfaces, lowers or increases the work function of the system, and promotes electron or hole accumulation in the organic semiconductor, resulting in pronounced substrate-mediated n-doping/p-doping. Our findings reveal a previously unrecognized environmental influence on ELA, establishing water as a key regulator of substrate-mediated interfacial energetics in organic electronic systems.

9:15am **LS-TuM-6 Investigation on Topotactic Phase Transition of $LaCoO_3$ Thin Films with in Situ XRD and Ambient Pressure Hard X-Ray Photoelectron Spectroscopy***, Hyunsuk Shin, Youngmin Yun,* Gwangju Institute of Science and Technology, Republic of Korea*; Okkyun Seo,* National Institute for Materials Science, Japan*; Seongeun Kim,* Chosun University, Republic of Korea*; Minsik Seo, Dongwoo Kim,* Gwangju Institute of Science and Technology, Republic of Korea*; Hojoon Lim,* Myongji University, Republic of Korea*; Hojun Oh, Subin Jang, Kyungmin Kim, Sae Hyun Kang,* Gwangju Institute of Science and Technology, Republic of Korea*; Adrian Hunt, Iradwikanari Waluyo,* Brookhaven National Laboratory*; Do Young Noh,* Gwangju Institute of Science and Technology, Republic of Korea*; Hyon Chol Kang,* Chosun University, Republic of Korea*;* ***Bongjin Simon Mun****,* Gwangju Institute of Science and Technology, Republic of Korea

To understand the correlation between the structure phase transition (SPT) and electronic/chemical properties of LaCoO3 (LCO), multimodal techniques, including in situ XRD, I-V measurement, and ambient pressure hard X-ray photoelectron spectroscopy (AP-HAXPES) are employed. Especially, AP-HAXPES not only allows operando analysis under wide pressure and temperature ranges, but also provides the direct bulk sensitive information of the electronic/chemical states. The AP-HAXPES measurement overcomes the difference of the probing depths between conventional XPS and XRD, thereby providing bulk-sensitive chemical/electronic structure information under reaction condition. The observed oxidation states in core level spectra, Co 2p, clearly showed that the oxygen vacancies play an important role in the SPT of LCO thin films. Importantly, the analysis of the valence band (VB) spectra of AP-HAXPES showed the presence of enlarged band gap formation, demonstrating the presence of the complex interplay between the oxygen vacancies and

electronic structure. The modified VB structures across the SPT are also compared to the in situXRD and transport measurements.

9:30am **LS-TuM-7 Advances in Hydrogen Technology Enabled by Synchrotron X-ray Methods***, **Nicholas Strange**,* SLAC National Accelerator Laboratory, United States Minor Outlying Islands (the) **INVITED**

Hydrogen energy represents a critical frontier in securing the United States' long-term energy resilience and global technological dominance. Achieving cheap, sustainable, and equitable hydrogen production at scale requires rapid advancement of the underlying materials science and process technologies, a challenge that has mobilized significant federal investment and a growing network of national laboratory partnerships. This talk will highlight previous and ongoing research within the materials science division at the Stanford Synchrotron Radiation Lightsource (SSRL), contextualized within the broader scopes of the HyMARC, H2NEW, H2NUC, HydroGEN, and HyBlend energy materials networks (i.e., DOE-led consortia uniting national laboratories around hydrogen production, storage, and transport).

The hydrogen R&D landscape is undergoing a decisive shift from foundational discovery toward application-focused development of materials optimized for specific performance and durability requirements. American leadership in this transition is essential, both to drive down the cost of clean hydrogen production and to establish the domestic industrial base necessary for long-term energy independence. *In situ* and *operando* X-ray scattering measurement designs developed at SSRL will be discussed, with results presented from a selection of collaborative projects aimed at accelerating this national effort.

Light Source Enabled Science
Room Ballroom A - Session LS-ThP

Light Source Enabled Science Poster Session

LS-ThP-1 Ultrafast Science at the NSF-NeXUS Facility, ***Seth Shields***, *John Beetar,* Ohio State University*; Conner Dykstra,* ohio state University*; Joohyung Park,* ohio State University*; TJ Ronningen,* ohio state University*; Robert Baker, Lou DiMauro, Jay Gupta, Roland Kawakami, Claudia Turro,* Ohio State University

The National Science Foundation (NSF) National eXtreme Ultrafast Science Facility (NeXUS) is a new open access user facility that provides access to extreme light to researchers around the world. The facility contains a mix of optical and analytical capabilities that allow for the study of chemical and material properties on the time scale of femtoseconds to attoseconds and on the length scale of angstroms. A customized high power, high repetition rate (800 W @ 100 kHz) Yb-doped fiber laser and pulse compression scheme from Active Fiber Systems GmbH is used to produce extreme ultraviolet light (XUV) through high harmonic generation. The XUV light is conditioned through three beamlines, which provide tailored light to a variety of end stations, three of which support materials analysis: X-ray absorption/reflection spectroscopy (XAS/XRS), Angle Resolved Photoemission Spectroscopy (ARPES), and Scanning Tunneling Microscopy (STM).

This poster will present the preliminary results and progress during the commissioning and inaugural user experiments at NeXUS.

LS-ThP-2 Operando Study of CO_2 Adsorption on PtGa (111) Surface, ***Subin Jang***, Gwangju Institute of Science and Technology, Republic of Korea*; Minsik Seo,* Nanyang Technological University, Singapore*; Hyunsuk Shin,* Samsung Electronics, Korea (Democratic People's Republic of)*; Dongwoo Kim,* KBSI, Republic of Korea*; Kyungmin Kim,* Gwangju Institute of Science and Technology, Republic of Korea*; Hojoon Lim,* Myongji University, Republic of Korea*; Jongkeun Jung,* Korea Institute of Science and Technology, Republic of Korea*; Dong Junf,* Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea*; Sung Yoo,* Korea Institute of Science and Technology, Republic of Korea*; Jeongjin Kim,* Pohang Accelerator Laboratory, Republic of Korea*; Lenart Dudy,* Synchrotron SOLEIL, France*; Jean-Jacques Gallet, Fabrice Bournel,* Sorbonne Université, France*; Bongjin Simon Mun,* Gwangju Institute of Science and Technology, Republic of Korea

Managing the surplus of CO_2 in Earth's atmosphere has become a critical global issue as it drives global warming and climate change. Consequently, many efforts are devoted not only on reducing CO_2 waste, but also on efficient conversion of CO_2 into valuable products. In this study, a PtGa (111) single–crystal alloy is used as a model catalyst to investigate surface chemical states under CO_2 using ambient–pressure X–ray photoelectron spectroscopy (AP–XPS). At 2×10^{-2} mbar CO_2 and room temperature, surface species assigned to carboxylate (CO_2^-) and carbonate (CO_3^{2-}) appear, indicating a clear pressure threshold for CO_2 adsorption on PtGa. When the surface temperature is raised under 0.2 mbar CO_2, the carboxylate signal disappears, while CO and carbonate intensify together with formation of GaO_x. During this process, only Ga is oxidized and Pt remains metallic, highlighting the key role of interfacial gallium oxide adjacent to Pt sites.

LS-ThP-3 Investigation Into Polymer Charge Localization with Soft X-Ray Absorption Spectroscopy, ***Jonathan Thurston***, University of Colorado at Boulder*; Shuya Li,* National Laboratory of the Rockies*; Qi Sun,* University of Arizona*; Dennis Nordlund,* Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory*; Luis Kitsu Iglesias, Collin Sindt,* University of Colorado at Boulder*; Santosh Kumar, David Grinter,* Diamond Light Source, UK*; Hong Li,* University of Arizona*; Ann Greenaway, Elisa Miller,* National Laboratory of the Rockies*; Michael Toney,* University of Colorado

Semiconducting polymers have sparked interest in electrochemical processes such as catalysis and energy storage due to their strong charge transport properties and ionic conductivity. Despite the importance of polymer-electrolyte interactions in device performance, there is a lack of understanding of the fundamental interphasial interactions that occur between the polymer and electrolyte. In this study, we use near-edge X-ray absorption fine structure spectroscopy (NEXAFS) and vibrational spectroscopy to study the local atomic electronic and chemical structure of a pi-conjugated redox active polymer. We use N2200, a well-studied polymer due to its high crystallinity, conductivity, and charge carrier mobility which has monomeric units consisting of an naphthalene diimide (NDI) with alkyl sidechains coupled with a bithiophene unit.

N2200 has two redox events correlating to the formation of polarons (-1 charge) and bipolarons (-2 charge) during charging that are accompanied by the absorption of counter-cations from the surrounding electrolyte for charge neutralization. We will introduce and discuss an *ex-situ* study in which carbon and oxygen NEXAFS is measured at different points in the polymer charging process and compare to an *operando* study in which the polymer charge is held potentiostatically while measuring NEXAFS. Using simulations, we assign electron excitation events to experimental NEXAFS spectra, identify polaron localization, and discuss how polymer-electrolyte interfacial interactions dictate charge transfer. Our results show how the charge localizes on the polymer and how elemental environments of the polymer change as a function of charge. This work addresses the impact of polymer choice as electrode materials on device performance and operation.

LS-ThP-4 Bridging Concept and Application: An LLM-Assisted Machine Learning Software Pipeline for Automated ARPES Analysis at MAESTRO, ***Sandy Adhitia Ekahana***, Carnegie Mellon University*; Hendrik Santoso Sugiarto,* Calvin Institute of Technology, Indonesia*; Chris Jozwiak, Aaron Bostwick, Eli Rotenberg,* ALS-LBNL*; Jyoti Katoch,* Carnegie Mellon University

Recent advancements in angle-resolved photoemission spectroscopy (ARPES) have enabled spatially resolved measurement, vastly increasing the dimensionality and complexity of the resulting multidimensional hyperspectral data. Processing this data creates a bottleneck, driving the need for automated techniques to label and map similar dispersion cuts spatially [1]. While self-supervised learning combined with k-means clustering can successfully automate these tasks [1], incorporating spatially-aware representations via graph convolution significantly enhances the transfer learning capabilities and classification accuracy for spatially resolved ARPES data [2]. However, translating these proven machine learning methodologies into practical, user-friendly software at experimental facilities like the MAESTRO beamline remains a critical challeng. This poster presents a fully functional Python application deployed for the MAESTRO beamline, transforming these advanced machine learning models [1, 2] into an accessible tool for general facility users. The software was developed from scratch using a Large Language Model (LLM)-assisted prompt-based generation approach, colloquially known as "vibe coding," utilizing Gemini-Pro. By leveraging a deep conceptual understanding of the analytical workflow and offloading the syntax generation to the AI, the application development was structured through deliberate, step-by-step prompting. The interface and underlying logic were built sequentially, one tab at a time. This methodological approach resulted in a highly modular architecture where the codebase is segmented into easily digestible chunks. This poster demonstrates both the underlying machine learning pipeline for ARPES data reduction [1, 2] and a modern, AI-assisted paradigm for rapidly prototyping and deploying robust scientific software.

[1] Ekahana, S. A., et. al. (2023). *Machine Learning: Science and Technology*, 4(3), 035021.

[2] Sugiarto, H. S., et. al. (2026). *Machine Learning: Science and Technology*, 7(2), 025007.

LS-ThP-5 Soft X-rays, Hard Questions: Identifying Band Character in Quantum Materials with ARPES, ***Jessica McChensey***, *Fanny Rodolakis,* Argonne National Laboratory, USA

We highlight the Intermediate Energy X-ray (IEX) beamline 29-ID at the Advanced Photon Source (APS), optimized for SX-ARPES with variable polarization, a near–magic-angle geometry that minimizes broadening and footprint, sub-10 K six-axis cryogenic manipulation, and integrated x-ray absorption (total/partial electron yield) alongside photoemission. The APS Upgrade extends the accessible photon-energy range to hv ≈ 184–2000 eV with increased flux, strengthening opportunities for bulk and buried-interface studies. I'll present several examples illustrating how the photon-energy dependence and polarization can be used to disentangle band character. For instance, in the heavy-fermion compound Ce2RhIn8, SX-ARPES suppresses problematic surface contributions and yields near-constant-kz momentum cuts, clarifying bulk Fermi-surface signatures in the low-temperature hybridized regime while revealing strong matrix-element effects that motivate matrix-element-aware modeling. In addition, circular dichroism SX-ARPES can be used to investigate the topology of the band structure. In the nodal-line semimetal ZrSiS, circular dichroism SX-ARPES reveals ~30% dichroism for both Dirac bands near the Fermi level and

deeper valence states, with sign reversals across crystallographic mirror planes.

LS-ThP-6 Palladium Nanofoams as a Framework for Hydrogen Storage, ***Alisson Steffli Thill,*** Universidade Federal do Rio Grande do Sul, Brazil*; Slavomir Nemsak,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Fabiano Bernardi,* Universidade Federal do Rio Grande do Sul, Brazil

Hydrogen has gained major attention as a renewable fuel, but efficient storage methods remain a challenge [1,2]. Metallic and oxide nanostructures have been explored to enhance hydrogen adsorption [3]. In a previous work of our group [4], it was demonstrated the possibility of synthesizing NiO nanofoams, which showed promising hydrogen storage performance under mild conditions compared to literature results. In part, this great performance is explained by the existence of the quasi-molecular bonding regime for the hydrogen adsorption process in NiO nanofoams. The quasi-molecular bonding of hydrogen with solid materials is the key factor for reaching the ultimate goal for hydrogen storage applications [5]. Considering the high hydrogen affinity of Pd and the promising adsorption results of NiO nanofoams, the development of Pd nanofoams has great conditions to display an even higher hydrogen storage performance.

In this work, the synthesis method was extended to produce Pd nanofoams using five phytantriol/water template phases. Therefore, five different Pd nanofoam samples were obtained. The samples were characterized by SEM, TEM, XRD, SAXS, AP-XPS, and AP-GIXS. Hydrogen adsorption measurements were also performed in order to obtain the hydrogen adsorption performance of all samples. Furthermore, DFT calculations were performed to determine the binding energy of hydrogen molecules in Pd structures.

For all samples, SEM and TEM images revealed Pd nanofoams composed of interconnected nanoparticles with diameters in the tens of nanometers range, forming channels of about 50-100 nm. The samples also contained isolated nanoparticles with diameters around 4 nm. XRD showed tunable fractions of metallic Pd and PdO. AP-XPS measurements before hydrogen exposure indicated an almost fully oxidized PdO surface, which rapidly reduced upon hydrogen exposure. Analysis of the AP-XPS data during hydrogen exposure showed that hydrogen interaction and Pd-H bond formation depend on the sample. These results can be correlated with theoretical calculations and sample morphology to explain the hydrogen adsorption performance.

References

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Acknowledgments

CNPq, CAPES, FAPERGS, ALS-LBNL, CNANO-UFRGS, CMM BR-Sul, CM-UFMG.

LS-ThP-7 Strain and Electronic Correlations in Metal-Insulator Transition of $CaVO_3$ Thin Films, ***Amitayush Jha Thakur,*** Argonne National Laboratory, India

The metal-to-insulator transition (MIT), which can occur as a function of temperature, pressure, doping, or applied bias, is a paradigmatic example of the dramatic consequences of strong electron correlations in solids and holds promise for new applications in the emerging field of Mottronics. $CaVO_3$ is metallic in bulk form and in thick films, but undergoes a pronounced MIT when the film thickness is reduced below 20 unit cells (u.c.). Unlike the MIT reported in ultrathin $SrVO_3$, this transition cannot be explained solely by dimensional crossover in thin films. Instead, the MIT in $CaVO_3$ appears to be mediated by a complex interplay of epitaxial strain, surface crystal-field splitting, and possible structural and magnetic transitions. Preliminary low-temperature measurements at 30 K on a limited set of samples reveal the electronic evolution of thin films across the MIT; however, systematic measurements across the full thickness and temperature range are still lacking. Here, we present a study of the electronic and structural properties of $CaVO_3$ thin films across this phase space using angle-resolved photoemission spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), and X-ray diffraction (XRD). These measurements allow us to investigate the drivers of the MIT and clarify the complex interplay between strain and electronic structure in this correlated oxide system.

LS-ThP-8 A NEXAFS Reference Library for Metal Compounds, *Matthijs A. van Spronsen, David C. Grinter, Pilar Ferrer,* ***Georg Held,*** Diamond Light Source, UK

Near edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy is an ideal tool to study materials under *in situ* and operando conditions. It gives quantifiable and element specific information on the oxidation state. As X-ray absorption can be measured in a variety of ways (transmission, electron and fluorescence yield), it can be more easily adapted to difficult experimental configurations than XPS. Typical NEXAFS analysis comprises comparing the experimental spectra to those of reference materials of know oxidation state and/or chemical structure. This procedure can be extended to linear combinations fitting of the spectra of interest. However, everything hinges on the availability of a set of reference compounds that capture the relevant chemistry. Currently, many hours of beamtime are used to measure the same readily available references by different user groups. This is ineffective use of beamtime and oftentimes the set of references does not include more exotic, potentially unstable, compounds. These are, however, critical for understanding materials under operating conditions because the *in situ* formed structure can be very different from the stable, well-known compounds.

At Diamond Light Source, we are in the process of building a comprehensive library of reference materials. The focus thus far has been on Co, Ni, and Ti compounds, and a total of 30 compounds have been measured including $Ni(OH)_2$, $LiNiO_2$, NiO, NiO_2, Ni_3S_2, CoO, Co_3O_4, $LiCoO_2$, $Co(OH)_2$, CoCO, and various Co and Ni metalorganics. These reference samples will be published in a public repository (GitHub) in an open access data format and viewable with an on-line data plotter. Furthermore, these will also be integrated in the control software used at Diamond (GDA).

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