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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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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