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Poster # - 30

An Enhanced Image Stitching Method for Atomic Force Microscopy

Arpan Biswas; Marti Checa Nualart; Liam Collins; Spencer Cox (Oak Ridge National Laboratory); Ruben Millan-Solsona (ORNL); Jennifer Morrell-Falvey; Huanhuan Zhao (University of Tennessee)

Atomic Force Microscopy (AFM) enables high-resolution imaging of material surfaces at the atomic scale, offering detailed insights into structural and functional properties. However, its limited scan area poses challenges in linking nanoscale features to macroscopic structures, particularly in applications like large-area composite analysis or dynamic change studies. To overcome this, it is necessary to acquire and stitch multiple small-range, high-resolution images into a seamless composite that retains accurate physical details. This requires a robust stitching tool capable of merging overlapping AFM images into a single, coherent, high-resolution mosaic. Conventional stitching methods, such as those based on features or Fourier transforms, often fail when dealing with images that are feature-sparse, minimally overlapping, or affected by complex transformations and noise artifacts. To address these limitations, we present an enhanced feature-based stitching approach, demonstrated using AFM images of biofilms formed by the bacterial strain Pantoea sp. YR343. Our method leverages domain expertise to select a feature-rich and correlated imaging channel (e.g., amplitude) to guide the alignment of a more challenging channel (e.g., topography). By using the correlated channel for feature detection and matching, we improve alignment accuracy and stitching performance. We compare our method with traditional direct stitching approaches and show that our technique significantly outperforms them. Further analysis reveals that computing the derivative of the topographical images along the x-axis produces features similar to those in the amplitude channel, enabling our method to generalize even in the absence of amplitude data. Although our focus is on AFM, the proposed strategy can be extended to optical microscopy by combining channels such as brightfield and fluorescence. We believe this multi-channel stitching workflow offers a powerful and generalizable solution for large-area microscopy image reconstruction and analysis.

Topical Area: AI and data science

Poster # - 36

Optimizing the Manufacturing of Inkless Printed Electronics with Machine Learning Models

Colton Bevel (Auburn University); Sumner B. Harris (Oak Ridge National Laboratory); Masoud Mahjouri-Samani; Adib Taba (Auburn University)

Best Student Presentation Award Entry

We present a machine learning approach for manufacturing printed electronics, enabling users to enter a target resistivity and receive optimized printing parameters to achieve it. The process is based on a dry additive nanomanufacturing (Dry-ANM) technique that produces pure nanoparticles via pulsed laser ablation. These particles are directed via argon through a nozzle and sintered in-situ onto a substrate. For this study, pure silver and copper were printed on a Polyamide substrate. Design of experiment algorithms were developed and optimized for incorporating new materials in the machine learning algorithm. Multiple machine learning models were trained to obtain relationships between process parameters and final resistivity. A search strategy study was then conducted using an ML algorithm to predict printing conditions with user-specified parameter ranges and target resistivity. Ultimately, it enables rapid and autonomous data-driven development of custom-printed electronics both on Earth and in space.

Topical Area: AI and data science

Poster # - 58

Machine Learning for Materials Study

Mariia Karabin (Postdoc); Wasim Raja Mondal (Postdoc); Hanna Terletska (Associate Professor)

Machine learning is emerging as a powerful tool to accelerate materials discovery across a wide range of chemical compositions and property spaces. In this work, we apply state-of-the-art machine learning techniques to two classes of functional materials: Heusler alloys and hybrid organic-inorganic perovskites (HOIPs).

Heusler alloys, discovered at the end of the nineteenth century, have emerged as exciting materials in the 21st century due to their fascinating properties, such as half-metallicity, martensitic transformation, and ferromagnetism. These properties make Heusler alloys promising candidates for applications in spintronics and thermoelectric devices. In this study, we aim to discover new Heusler alloys using state-of-the-art machine learning approaches.
Our dataset includes 423 distinct X_2YZ ternary full Heusler compounds, where X and Y are transition metals (from the d-block of the periodic table), and Z is a main-group element. We apply supervised machine learning methods—including Kernel Ridge Regression (KRR), Support Vector Machines (SVMs), Random Forest, and Gaussian Process Regression—to model and predict the formation energy of new Heusler alloys.

Among these models, KRR demonstrates the highest accuracy for our dataset. After validating the model, we use it to predict new Heusler alloys. Our study provides valuable insights that can guide both computational screening and experimental synthesis of novel Heusler materials. In parallel, we also explored dimensionality prediction in hybrid organic-inorganic perovskites (HOIPs), where dimensionality plays a critical role in determining the material's electronic properties, optical, and stability. Using a curated dataset of experimentally synthesized HOIPs, we extract a set of descriptors as well as add engineered features to improve model accuracy and generalization. A classification model is trained to predict 0D, 1D, 2D, and 3D structural dimensionality, enabling high-throughput screening of candidate HOIPs. This predictive model facilitates the design of perovskites with targeted dimensionality.

Topical Area: AI and data science

Poster # - 74

Cloud Processing and Direction of Automated and Autonomous Characterization using Piezoresponse Force Microscopy

Ralph Bulanadi (CNMS) Sumner B. Harris (Oak Ridge National Laboratory); Yongtao Liu (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Rama Vasudevan

Best Student Presentation Award Entry

Automated and autonomous experiments can revolutionize scientific discover—such "labs of the future" process vast amounts of scientific data and use this knowledge to inform and direct on-the-fly experiments. However, the application of such rapid, computationally intensive data processing steps can be severely limited by hardware and processing speed, particularly where computer systems are designed primarily for machine operation.

To facilitate future self-driven experiments, allow new levels of cross-facility collaboration, and expand user capabilities, we have integrated three software ecosystems developed at ORNL and CNMS to enable cloud-directed autonomous experiments. Instrument-control software (AEcroscopy) is used to operate a commercial atomic force microscope to measure and characterize a model ferroelectric sample. A cross-facility orchestration software ecosystem (INTERSECT-sdk) is then used to transmit measurement updates and file locations to a cloud server, on which a machine learning package (GPax) is used to process the new experimental data and transmit new experimental parameters back to AEcroscopy via INTERSECT-sdk.

Such development, here used to investigate local switching behavior, presents a model for labs of the future, where data sourced from different machines, computers, or even facilities can be collated, processed, and utilized for future high-throughput autonomous experiments.

Topical Area: AI and data science

Poster # - 96

NDIP and NOVA: Workflows and Interfaces for Neutron Scattering

Andrew Ayres Gregory Cage (Oak Ridge National Laboratory); John Duggan (Oak Ridge National Laboratory); Greg Watson (Oak Ridge National Laboratory); Sergey Yakubov (Oak Ridge National Laboratory)

Neutron Scattering workflows are a core part of daily operations for SNS and HFIR scientists at Oak Ridge National Laboratory (ORNL). However, there can be challenges relating to the ease of access, use, and reproducibility of these workflows. We have developed the Neutron Data Interpretation Platform (NDIP) and the Neutrons Open Visualization and Analysis (NOVA) framework to tackle these challenges. NDIP and NOVA provide scientists with the tools to create web based user interfaces (UIs) and take advantage of computational resources, advanced visualization tools, and reproducible analysis pipelines.

NDIP is built around the open-source Galaxy project, a web-based scientific workflow engine and UI, built to enable scientists to easily manage data, create workflows, and simplify the reproduction of past results. Our efforts have integrated our own Galaxy instance, Calvera, with various computational resources including Frontier at ORNL and Perlmutter at NERSC. Calvera handles the authentication, the submission, and the reporting of results from these resources.

The NOVA framework was designed to enable scientists to develop custom UIs that take advantage of NDIP's capabilities to run workflows and tools. NOVA provides tools to create Model-View-ViewModel applications utilizing a variety of front–end technologies including Trame, Panel, and QT. Scientists can also use NOVA to launch jobs through NDIP, run workflows, retrieve their results, and display them in their interfaces.

Our poster will highlight the work done on both NDIP and NOVA, describe their capabilities, and show examples of how NDIP and NOVA have facilitated the development of Neutron Scattering workflows and interfaces.

Topical Area: AI and data science

Poster # - 102

Commissioning on-the-fly, autonomous neutron diffraction experiments for exploring spin flop transitions for α-Fe2O3

Marshall McDonnell (Oak Ridge National Laboratory) Andrew Ayres (Oak Ridge National Laboratory); Gregory Cage (Oak Ridge National Laboratory); Luke Daemen (Oak Ridge National Laboratory); Stephen DeWitt (Oak Ridge National Laboratory); Mathieu Doucet (ORNL); Lance Drane (Oak Ridge National Laboratory); Kaz Gofron; Amy Gooch; Ray Gregory (Oak Ridge National Laboratory); Gilad Kusne (National Institute of Standards and Technology); Paul Laiu (Oak Ridge National Laboratory); Jue Liu (Oak Ridge National Lab); Addi Malviya-Thakur (Oak Ridge National Laboratory); Jack Marquez (University of Tennessee); Austin McDannald (National Institute of Standards and Technology); Kin Hong NG (University of Tennessee); Valerio Pascucci (University of Utah); William Ratcliff (NIST); Giorgio Scorzelli (University of Utah); Ankit Shrivastava (Oak Ridge National Laboratory); Michela Taufer (University of Tennessee Knoxville); Zach Thurman (Oak Ridge National Laboratory); Matthew Tucker; Bogdan Vacaliuc (Spallation Neutron Source); Emily Van Auken (Oak Ridge National Laboratory); Greg Watson (Oak Ridge National Laboratory); Yuanpeng Zhang (ORNL)

The Experimental Steering for Powder Diffraction (ESPD) project aims to help develop and commission automation and steering neutron powder diffraction experiments. Recently, successful experiments on the Nanoscale-Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source (SNS) were conducted for the ESPD project and results will be presented. Specifically, iron(III) oxide / hematite (α-Fe2O3) bulk and nanoparticles were measured using NOMAD's cryostream for autonomous navigation of temperature measurements via machine learning (ML) to commission experiment steering capabilities. Two methods were used for the ML decision making for new temperatures: a Bayesian optimization method and a physics-informed method called ANDiE (Autonomous Neutron Diffraction Explorer) developed previously by a team from National Institute of Standards and Technology (NIST). The experiment used the Morin temperature / spin flop transition of α-Fe2O3 to autonomously explore using both methods. The ML methods were developed and deployed via the Distributed Interconnected Science Ecosystem INTERSECT) for Active Learning (DIAL) project. The Data Acquisition Group's External Instrument Control (EIC) software was used to securely "talk" to the NOMAD EPICS system to change the temperature of the cryostream and used a combination of INTERSECT ad DIAL services to steer the NOMAD instrument. The data was streamed to a separate instance of INTERSECT running in the National Science Data Fabric for visualization of progress of the experiment. This work provides a foundation to drive progress towards both large-scale compute resources being used to guide experiments at SNS and HFIR as well as promote and mature this capability for the General User Program instead of as one-off, proof-of-concept experiments. The future scientific impact from this study will be significant reduction in experimental time required for neutron diffraction experiments and better exploration of parameter space with the constraint of finite beamtime for Users.

Topical Area: AI and data science

Poster # - 114

Building Automated PFM Scientist

Kamyar Barakati (University of Tennessee Knoxville); Sergei Kalinin; Richard Liu (University of Tennessee Knoxville); Aditya Raghavan (University of Tennessee Knoxville)

Ferroelectric materials exhibit diverse behaviors influenced by local structure, domain configurations, and external stimuli. To support their systematic exploration, an integrated platform has been developed that combines autonomous scanning probe microscopy (SPM), physics-informed measurements, and machine learning-guided decision-making.

In one study, domain wall dynamics in $PbTiO_3/KTaO_3$ heterostructures are investigated. Global SPM scans are used to identify candidate regions, followed by autonomous selection of areas containing specific domain wall types. Voltage pulses with varying amplitude and duration are applied in a controlled, repeatable manner across hundreds of sites. This enables statistically robust, spatially resolved insights into domain wall mobility and switching behavior.

In a separate investigation, automated DART-PFM is used to characterize ferroelectric responses in composition-spread libraries, including Sm-doped $BiFeO_3$ (SmBFO) and $Al_{1-x-y}B_xSc_yN$ (AlBScN). High-throughput maps of polarization loops, piezoresponse strength, and domain morphology are obtained. The morphotropic phase boundary in SmBFO is localized, and previously unreported functional transitions are identified in AlBScN.

To enable data-driven materials optimization, a multi-objective Bayesian optimization framework based on deep kernel learning (MOBO-DKL) is implemented. Domain-specific reward functions—such as loop area, net piezoresponse, and domain symmetry—are used to guide measurement selection. Pareto front analyses support simultaneous optimization of competing objectives and discovery of regions with desired functional responses.

Topical Area: AI and data science

Poster # - 120 (Wednesday CNMS Poster Session)

Agentic AI Empowered Hub Soft Materials Synthesis for Functional AM

Ilia Ivanov, Rama Vasudevan, Bobby Sumpter, Panos Christakopoulos, Junqi Yin, Emily Herron, Monojoy Goswami and Gobet Advincula

Abstract AI-centric multimodal testing of materials (IMES) coupled to autonomous synthesis **AUTOflowS** platform, empowered by theory and simulation, coupled through RAG-LLM interface and assisted by a digital twin could come together in a powerful R&D tool kit enabling workflows for accelerated materials discovery and unfolding origins of structure- functional dependencies which are critical for energy applications.

Acknowledgement This effort was funded by Intersect LDRD program and conducted at the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory

Topical Area: AI and data science

Poster # - 13

Analyzing the dynamics of the Nsp13 helicase in the SARS-CoV-2 replication-transcription complex

Gregory Hura (LBNL); Sharique Khan (ORNL); Wellington Leite (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Susan Tsutakawa (LBNL); Jennifer Warnock (ORNL); Qiu Zhang

At around 30 kb, the SARS-CoV-2 genome is one of the largest viral genomes among RNA viruses. As such, the replication machinery must be prepared to quickly and efficiently replicate this genome in order for the viral infection to effectively persist. The SARS-CoV-2 replication-transcription complex (RTC) involves several non-structural proteins encoded by the viral genome that accomplish this goal. The complex includes the RNA-dependent RNA polymerase (RdRP) Nsp12, the helicase Nsp13, and the cofactors Nsp7 and Nsp8, which assemble with RNA to form the RTC. While there are some structures of the replication-transcription complex (RTC) that show the stoichiometry of the proteins and their location within the complex, there still remain some questions about the dynamics of these proteins in complex. One of the remaining questions regards the dynamics of Nsp12 and Nsp13 with RNA, as the placement of these in complex and the directionality of the polymerase and helicase activities seem to be at odds. One explanation for this could be that the helicase allows for backtracking of the RNA in case of a polymerase mistake. By performing SEC-SAXS on different components of the RTC complex, we hope to elucidate the dynamics of these different proteins with each other and with RNA.

Topical Area: Biology and life sciences

Poster # - 15

Automated AFM for Large-Area Biofilm Imaging and Characterization of Antifouling Surfaces

Ruben Millan-Solsona (ORNL) Spenser R. Brown; Martí Checa; Sita Sirisha Madugula; Lance Zhang; HuanHuan Zhao; Amber Webb; Nickolay V. Lavrik; Rama Vasudevan; Arpan Biswas; Scott Retterer; Jennifer L Morrell-Falvey; Liam Collins

Biofilms are complex microbial communities encased in an extracellular matrix, exhibiting structural and functional heterogeneity driven by chemical and nutritional gradients. Their architecture enhances resilience and antibiotic resistance, posing challenges in clinical and industrial contexts. Traditional analysis methods often lack the spatial resolution and contextual integrity needed to capture their full complexity.

To overcome these limitations, we developed an automated platform for large-area Atomic Force Microscopy (AFM) imaging, capable of high-resolution mapping over millimeter-scale regions. Combined with image stitching and machine learning-based analysis, our approach preserves spatial relationships and reveals key biofilm features, including cellular arrangements, and flagella.

We applied this platform to study Pantoea sp. YR343 biofilms on gradient-structured and antifouling surfaces, revealing how surface properties influence biofilm morphology and stability. In particular, we observed a honeycomb architecture on hydrophobic regions and demonstrated the role of flagella in structural integrity. By automating AFM imaging, we extend its applicability to mesoscale investigations, offering a powerful tool for characterizing biofilm-surface interactions and advancing the design of antifouling materials.

Topical Area: Biology and life sciences

Poster # - 37 (Wednesday CNMS Poster Session)

Structural Characterization of Lipid Nanoparticles Using Deuterated Ionizable Lipid SM-102

Brandon Nusser (Oak Ridge National Lab)

We report the synthesis of deuterated ionizable lipid SM-102 (13 steps, 96% deuteration). Empty and RNA loaded lipid nanoparticles, composed of deuterated SM-102, 1,2-distearoyl-sn-glycero-3-phosphocholine, cholesterol, and 1,2-dimyristoyl-rac-glycero-3-methoxypolyethylene glycol-2000, are synthesized using a syringe pump and a microfluidic chip. The particle size, uniformity, and internal structure of the lipid nanoparticles are characterized by dynamic light scattering, small angle x-ray scattering, and small angle neutron scattering experiments. The syringe pump and microfluidic chip yield small, monodispersed particles, due to the control of flowrate and mixing. Scattering experiments are consistent with a core-shell structure.

Topical Area: Biology and life sciences

Poster # - 43

Effects of central dogma processes on the compaction and segregation of bacterial nucleoids

Jan Michael Carrillo (ORNL); Mu-Hung Chang (University of Tennessee); Maxim Lavrentovich; Jaan Mannik

Best Student Presentation Award Entry

The bacterial cytoplasm is characterized by a distinctive membrane-less organelle, the nucleoid, which harbors chromosomal DNA. We investigate the effects of dynamic processes associated with transcription and translation on the structure of this organelle, using coarse-grained molecular dynamics (MD) simulations implemented through the LAMMPS package and its recently developed REACTER module. Our model captures the scale of the entire cell and incorporates a reaction-diffusion system for ribosomes and polyribosomes, integrating their dynamics with DNA through excluded volume interactions and out-of-equilibrium processes. Our findings demonstrate that out-of-equilibrium processes generate distinct local microscopic structures within the nucleoid while reducing overall DNA compaction. Furthermore, we find these processes are essential for complete sister chromosomes separation and the establishment of the quarter positioning pattern of each nucleoid, which has been observed experimentally.

Topical Area: Biology and life sciences

Poster # - 51

Biosynthesis of Deuterated Lipids for Characterization of Biomembranes and Membrane Proteins

Qiu Zhang (Oak Ridge National Laboratory) Alan Hicks (Oak Ridge National Laboratory); Wellington Leite (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Sai Venkatesh Pingali (Oak Ridge National Laboratory); Volker Urban (Oak Ridge National Laboratory); Kevin Weiss; Honghai Zhang

Membrane proteins play crucial roles in many cellular processes, however, studying membrane proteins is challenging because of their complex structure and fragility when isolated from their native environment. One solution is to embed membrane proteins in a membrane-mimic to provide a more native environment to facilitate their characterization. Small-angle neutron scattering (SANS) is an ideal technique to obtain structural information on biomacromolecules under physiologically relevant conditions. With this technique, deuterated phospholipids need be used to suppress their 1H signal in SANS measurements. In this study, we report on producing deuterated phosphatidylethanolamine (PE) by extraction and fractionation from native Escherichia coli extracts, and phosphatidylcholine (PC) from an engineered E. coli strain. The regiospecific deuterium incorporation of PC can be controlled by growth conditions. The isolated PC product was confirmed by 1 H Nuclear Magnetic Resonance (NMR) and Liquid Chromatography - Mass Spectrometry (LC-MS) was used as a complementary tool for SANS to predict deuteration levels. These materials can be used for neutron scattering studies with micelles, bicelles, liposomes, styrene-maleic acid lipid particles (SMALPs), and Membrane Scaffold Protein (MSP)-based lipid nanodiscs to produce a membrane-mimicking environment for studying membrane proteins, and can be used for lipid studies using NMR as well.

Topical Area: Biology and life sciences

Poster # - 57 (Wednesday CNMS Poster Session)

Deuteration of Molecules and Macromolecules

Honghai Zhang, Peter Bonnesen; Wellington Leite (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Qiu Zhang

Small-angle neutron scattering (SANS) has become a very powerful technique to obtain structural information of polymers, functional organic materials and biomolecules. With this technique, different kinds of deuterated molecules are needed to obtain a high signal-to-noise ratio and selectively highlight the desired parts in complex system. In recent work, we synthesized several deuterated monomers, lignin, ionizable lipids and phosphatidylcholine for SANS studies. To shorten the synthetic period of deuterated molecules, we also established a deuteration platform for amines and amides, which are key precursors of many polymers, biomolecules and drug molecules. These works will enhance our deuteration capability and attract more users for neutron experiments

Topical Area: Biology and life sciences

Poster # - 65

Toxic Effects of Biofuel Molecules on Membrane Domains as an Unrecognized Mode of Cell Stress

Luoxi Tan; Jonathan Nickels (University of Cincinnati) Micholas Dean Smith; Sai Venkatesh Pingali; Hugh O'Neill (Oak Ridge National Laboratory); John Katsaras; Jeremy C. Smith; Brian H. Davison

Solvent toxicity represents an upper limit on fermentation titer and yield. This co-solvent induced stress occurs as amphiphilic co-solvent molecules partition into membrane, leading to membrane thinning, destabilization, and ultimately cell death. However, such stress does not fully account for the effect on the lateral membrane organization. In this study, we utilized small angle neutron scattering and molecular dynamics simulations to investigate the effect of n-butanol on transverse and lateral membrane structure. N-butanol is an important biofuel and biobased chemical precursor which can be produced through fermentation. Our studies demonstrated the extent of n-butanol partitioning, solvent induced membrane thinning, and solvent induced changes to the size of membrane domains. Parallel simulations proved a clear mechanism connecting membrane transverse structure, solvent partitioning and changes to line tension at the membrane domain boundaries. As the line tension increases, membrane domains appear to coalesce into fewer, larger domains to minimize the interfacial length – if one assumes constant domain area. We also observe significant structural disorder at the domain interface. Both observations represent unrecognized modes of membrane / solvent associated cell stress which may represent new directions to improve microbial solvent tolerance.

Topical Area: Biology and life sciences

Poster # - 77

Non-ideal mixing drives complex micellization morphology and phase behavior of mixed nonionic surfactants

Andrea Perez (University of California Santa Barbara) Raphaële Clement (University of California Santa Barbara); Glenn Fredrickson (University of California Santa Barbara); Leo Gordon (University of California Santa Barbara); Matthew Helgeson (UC Santa Barbara); Scott Shell (University of California Santa Barbara); David Zhao (University of California Santa Barbara)

Best Student Presentation Award Entry

There is considerable interest in replacing perfluoroalkyl surfactants (PFAS) with more environmentally benign substitutes in a range of industrial and consumer applications. Since individual alkyl and silicone-based surfactants consistently underperform against PFAS, mixtures of surfactants are being considered as potential substitutes. In many cases, property data are interpreted assuming that chemically homologous co-surfactants completely mix at the molecular scale, often with ideal mixing thermodynamics. However, limited studies with co-surfactant mixtures involving large differences in spontaneous curvature lead to a number of non-ideal phenomena including non-monotonic mixture phase behavior and complex assembled structures in solutions and emulsions. To better elucidate the molecular origins of this behavior we report combined structural, thermodynamic, and chemical characterization in model mixed ethoxylated alkane (CiEj) co-surfactants in aqueous solutions (water/surfactant). Phase behavior and calorimetric studies in these mixtures exhibit a significant non-monotonic dependence of critical temperatures and micellization thermodynamics that indicate non-ideal mixing in co-surfactants with disparate spontaneous curvature (e.g., C12E5/C4E1) relative to geometrically similar co-surfactant pairs (e.g., C12E5/C12E6). Using a combination of viscometry, dynamic light scattering (DLS), and contrast-variation small angle neutron scattering (CV-SANS) measurements to resolve micelle morphology and intermolecular interactions, we show that this behavior corresponds with significant temperature-dependent differences in solvation between the mixed surfactants and their pure component counterparts. Ultimately, we hypothesize that differential solvation structures between co-surfactants in the mixed state provide a potential explanation for all the observed non-ideal behavior, and we test this hypothesis against molecular dynamics and field-theoretic simulations.

Topical Area: Biology and life sciences

Poster # - 78

CLAMPS Substrates Support Ex Vivo Axon Extension from the Hypothalamus in Brain-on-Chip Platforms

Brenna Ellis (University of Tennessee, Knoxville); Josh Hillner (University of Tennessee, Knoxville); Jake Lockhart (University of Tennessee, Knoxville); Larry Millet (University of Tennessee, Knoxville)

Over the past 17 years, nearly 600 publications have explored microfluidic platforms or tissue chips for localized drug perfusion and electrophysiological monitoring of organotypic brain slices. However, only a few studies report actual axonal projections from these slices. Achieving axonal outgrowth in microfluidic systems has remained difficult and is often deemed infeasible in peer review. Among successful cases, the hippocampus is key—its structure offers a natural edge, allowing dissection with minimal damage and preserving axonal architecture. To date, no other brain region has demonstrated ex vivo axonal extension in organotypic slices.

The hypothalamus, essential for physiological homeostasis, poses unique challenges due to its complex architecture and lack of defined axonal exit zones. Magnocellular neurons from this region are particularly resistant to survival and outgrowth in standard culture.

In this work, we present a microfluidic and surface chemistry strategy enabling axonal extension from hypothalamic organotypic brain slices. Our custom surface formulation, called CLAMPS (Cell-Like-Adhesion through Matrix-Polymer Substrates), combines peptide epitopes with carbon-based aliphatic polymers to create a transparent, molecular-scale substrate. CLAMPS in microfluidics rescues magnocellular neurons from failure-to-thrive conditions in dishes and microfluidic cultures.

We demonstrate that CLAMPS is necessary and sufficient to support magnocellular neuron growth in monoculture compared to standard conditions ($p < 0.0001$, one-way ANOVA with multiple comparisons). CLAMPS-based microfluidics also sustain hippocampal organoids and retain brain slice integrity in vitro.

Microfluidic devices were fabricated at CNMS-NRL (CNMS2024-B-02677) using SU-8 photolithography and PDMS molding. Chambers are 300–400 μm tall, with 50 μm channels supporting axonal conduit formation and localized perfusion. Axonal outgrowth from hypothalamic biopsy punches was confirmed in 5-week-old brain slices cultured for 10 days, then immunolabeled for axonal tau.

Topical Area: Biology and life sciences

Poster # - 85

Advancing Liquid Handling Capabilities at Bio-SANS

Kevin Weiss; Sai Venkatesh Pingali; Wellington Leite (Oak Ridge National Laboratory); Alan Hicks (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory)

Liquid handling capabilities at the Bio-SANS beamline are being advanced through a combination of sample environment developments. Continuous flow size-exclusion chromatography SANS (SEC-SANS) is now available to support in situ separation of complex samples, reducing aggregation and enabling analysis of labile species. A stopped-flow capability and a robotic pipetting system are also under active development to support time-resolved studies and automated sample preparation respectively. These efforts aim to broaden experimental possibilities as well as improve the consistency and reliability of sample handling for biological SANS studies.

Topical Area: Biology and life sciences

Poster # - 87

Small-Angle Neutron Scattering Reveals Extended Conformations in Electron-Bifurcating ETF

Sharique Khan; Alan Hicks (Oak Ridge National Laboratory); Wellington Leite (Oak Ridge National Laboratory); James Byrnes (Brookhaven National Laboratory); Biswajit Gorai (Technische Universität Berlin); Maria-Andrea Mroginski (Technische Universität Berlin); Hugh O'Neill (Oak Ridge National Laboratory); Anne-Frances Miller (University of Kentucky)

Electron bifurcation enables energy conservation in biological systems by coupling exergonic and endergonic redox reactions. In bifurcating electron transfer flavoproteins (Bf-ETFs), a large-scale conformational rearrangement is thought to gate electron flow by positioning flavins to enable or prevent inter-flavin transfer. However, the conformational ensemble sampled in solution has remained poorly understood. Here, we combine small-angle neutron scattering (SANS), small-angle X-ray scattering (SAXS), and advanced molecular modeling to probe the solution conformations of the bifurcating ETF from Acidaminococcus fermentans (AfeETF). Our SANS data reveal a dominant population of extended conformations in oxidized ETF, with radii of gyration ~4 Å larger than any known crystal structures, comprising over 50% of the ensemble. Reduction of flavins shifts the equilibrium toward more compact states, as validated by both NADH and dithionite-treated samples. Using ensemble optimization via a genetic algorithm informed by over 1,600 conformations generated from Bilbo-MD and metadynamics simulations, we achieve excellent agreement with SANS data. Contrast variation SANS experiments with selectively deuterated partner protein (BCD) further support conformational remodeling upon complex formation. These results challenge the static two-state model of ETF dynamics, proposing instead a spectrum of accessible conformations where extended forms act as structural intermediates linking the canonical "open" and "closed" states during catalytic turnover. This work establishes solution-phase structural dynamics as a critical component of electron bifurcation and highlights SANS-guided ensemble modeling as a powerful strategy for elucidating functionally important protein motions.

References:

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Topical Area: Biology and life sciences

Poster # - 89

Upgrades to the reduction and data analysis pipeline at Bio-SANS

Alan Hicks (Oak Ridge National Laboratory) Wellington Leite (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Sai Venkatesh Pingali; Yingrui Shang (ORNL)

Reduction and subsequent data analysis are the two fundamental steps to interpreting small angle neutron scattering data. At Bio-SANS, we have developed new analysis tools to streamline the data reduction and primary data analysis workflows. We have developed a new interactive, web-based analysis tool for solution scattering of biomolecules and extensible to soft matter polymer samples that provides interactive background subtraction integrated with pair distance distribution function calculation, Kratky and Guinier plots. The tool allows for quick interpretation of background subtracted data. We have also developed a new ensemble optimization genetic algorithm for SANS data to interpret SANS of flexible biomolecular systems. We have collaborated with SIBYLS beamline at ALS to host the genetic algorithm as part of the BilboMD workflow, for fast sampling of conformational space. In addition, we will present an overview of the future plans to improve the data pipeline at Bio-SANS, including live-data reduction, expansion of structure based contrast prediction (SCOMAP-XD), and multi-modal refinement with SAXS data.

Topical Area: Biology and life sciences

Poster # - 92

Sustained Autobioluminescence In Glioblastoma Cells Via Microfluidic Culture And Synthetic Promoter Optimization

Lisa Amelse (University of Tennessee, Knoxville); Tingting Xu (University of Tennessee, Knoxville); Jake Lockhart (University of Tennessee, Knoxville); Larry Millet (University of Tennessee, Knoxville)

Glioblastoma multiforme (GBM) is the most aggressive and lethal primary brain malignancy, characterized by diffuse infiltration, treatment resistance, and profound molecular heterogeneity. Despite intensive tri-modal therapy—surgery, radiation, and temozolomide—median survival remains just 15 months, underscoring the need for more predictive models and novel therapies. Bioluminescence imaging (BLI) is a biotechnology for tracking tumor progression in vivo, but conventional systems require repeated luciferin administration, limiting consistency and temporal resolution. To overcome this, we engineered a codon-optimized, self-illuminating synthetic lux operon (pLux) for stable autobioluminescence in mammalian cells, eliminating substrate dependence.

To enable early, ethical, and scalable testing of such biosensors, we developed a microfluidic tumor-on-a-chip platform that offers a cost-effective, preclinical validation of the autobioluminescent cell models. We designed a microporous membrane-based microfluidic bioreactor—referred to as a microfluidic tumor reactor—to serve as a continuous perfusion system for autobioluminescent glioblastoma cells. This platform was developed to overcome confounding premature downregulation of bioluminescent signals observed in conventional static culture systems. Signal downregulation was hypothesized to arise from microenvironmental deterioration, particularly nutrient depletion and/or metabolic waste accumulation, conditions that may contribute to transcriptional silencing or degradation of the pLux cassette. By enabling continuous perfusion and selective molecular exchange across a semipermeable membrane, the microfluidic reactor maintains a more physiologically relevant nutrient-waste balance and supports long-term culture viability to resolve reporter signal fidelity.

With the observations in microfluidics, the existing viral origin (CMV) promoter in our synthetic lux construct, was exchanged for a chicken β-actin (CAG) promoter to drive synthetic lux expression. The CAG promoter was amplified to generate the construct pCAG-Lux in E.coli, it was then isolated, transfected, and tested in GBM cells to achieve more than three-times the duration of autobioluminescence in vitro.

Topical Area: Biology and life sciences

Poster # - 100

Recent Advances of the Center for Structural Molecular Biology

Felicia Gilliland (Oak Ridge National Laboratory); Alan Hicks (Oak Ridge National Laboratory); Wellington Leite (Oak Ridge National Laboratory); Sai Venkatesh Pingali; Volker Urban (Neutron Scattering Division, ORNL); Kevin Weiss; Honghai Zhang; Qiu Zhang

The Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory (ORNL) is a national user facility funded to support and develop the user access and science research program of the Biological Small-Angle Neutron Scattering (Bio-SANS) instrument at the High Flux Isotope Reactor (HFIR) dedicated to the analysis of the structure, function and dynamics of complex biological systems and the Bio-Deuteration Laboratory for expression and purification of deuterium labeled biomacromolecules and for synthesis of small molecules and ligands in support of the biology neutron scattering program. This resource complements capabilities at other Department of Energy (DOE) Office of Biological and Environmental Research (OBER) facilities for structural biology. The CSMB supports a vibrant biological research community from academia, industry, and government laboratories.

Topical Area: Biology and life sciences

Poster # - 10

Uncovering Bias and Underestimated Errors in Neutron Diffraction Residual Strain Measurements

Cole Franz (The University of Tennessee, Knoxville) Jeffrey Bunn (Oak Ridge National Laboratory); Katharine Page (The University of Tennessee, Knoxville); Andrew Payzant (Oak Ridge National Laboratory); Michael Prime (Los Alamos National Lab)

Best Student Presentation Award Entry

Typical one-standard-deviation measurement uncertainties in neutron and x-ray diffraction may often fail to account for the complexity of residual strain fields in additively manufactured components. In these methods, measured strains are collected at multiple orientations to describe an underlying strain tensor. However, when only a few measurements are used or the model is overly simplified, the resulting solution may deviate systematically from ground truth. In addition, uncertainties may be underestimated. In such cases, the stability (invariance) and systematic deviation (bias) of the solution cannot be assessed without collecting more data than the minimal inverse solution requires. This research demonstrates how bias and variance are evaluated when calculating strain tensors with complex strain states, using data collected from a solid-state additive component via neutron diffraction. Bias, which is typically unknowable, can be evaluated in this special case, since each measured strain must satisfy common strain transformation. In addition, the analysis will be extended to a reference sample (i.e., ring-and-core) with a known stress state to demonstrate that this phenomenon of underestimated uncertainties is generalizable to the broader neutron diffraction / residual stress community. Suggestions based on the critical number of measurements needed to evaluate systematic effects (underestimated uncertainty) will be made based on the analyses of both the additive and reference samples.

Topical Area: Emerging research and multimodal techniques

Poster # - 28

Small-Angle Neutron Scattering Instrument Concepts for Second Target Station of SNS

Shuo Qian (ORNL)

Small-Angle Neutron Scattering (SANS) is a powerful and popular technique widely used for structural characterization in many science and engineering fields. The Second Target Station (STS) of the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) has been specifically designed to provide a broad bandwidth, high-brightness cold neutron source that is ideally suited for SANS instruments. Along with the advancements in neutron optics and computational algorithms, STS maximizes the potential of future SANS instruments at ORNL to provide the user community with unprecedented capabilities. For example, users will be able to perform experiments with ten times less sample, simultaneously measure phenomena at both atomic and mesoscopic scales, and investigate sub-second kinetic processes under in situ/operando conditions.

In this presentation, the current instruments under development are introduced as follows:

CENTAUR, the most developed, is a versatile workhorse in its preliminary design phase. It offers simultaneous wide-angle and diffraction coverage, catering to diverse fields from soft matter to quantum sciences. Still in concept, FocuSANS prioritizes high throughput for rapid, sub-second kinetic studies, ideal for dynamic processes or limited samples. Lab-On-SANS, another concept, focuses on real-world processing, allowing in situ microstructure measurements during processes like additive manufacturing. Finally, Auto-SANS, also conceptual, will integrate AI and robotics for autonomous sample synthesis, characterization, and analysis, even incorporating multi-modal techniques like X-ray scattering for comprehensive insights.

Topical Area: Emerging research and multimodal techniques

Poster # - 32

Observing Partial Order of the Random Hydrogen Network in Ice Ih

Tianran Chen (University of Tennessee, Knoxville); David Tennant (University of Tennessee, Knoxville) Isaac Ownby (University of Tennessee, Knoxville); Arnab Banerjee (Oak Ridge National Laboratory); Anjana Samarakoon (Oak Ridge National Laboratory); Johnathan Morris (Xavier University); Feng Ye (Oak Ridge National Laboratory); Douglas Abernathy (Oak Ridge National Laboratory); Zachary Morgan (Oak Ridge National Laboratory); Bastian Klemke (Helmholtz Center for Materials and Energy - Berlin); Konrad Siemensmeyer (Helmholtz Center for Materials and Energy - Berlin); Joseph Lanier (Xavier University)

Best Student Presentation Award Entry

In the condensed phase, water ice contains a well-ordered lattice of Oxygen atoms that hosts a disordered network of Hydrogen atoms. At ambient pressure, water ice (Ih phase) has a hexagonal crystal structure, reflected geometrically in the 6-fold symmetry of snowflakes. The transition from ice Ih to ice XI, the most stable phase, is expected to occur at time-scales of ~10,000 years. The hydrogen atoms in *pure* water ice have not been observed to order at low temperatures under ambient pressure. The predominant theory of ice assumes that the Hydrogen dipole moment dominates interactions. We observe hidden strings of 1D order within the disordered manifold of hydrogen atoms, revealed via optical phonons within a large multi-dimensional neutron scattering dataset. Our analysis shows that nearest-neighbor intermolecular interactions drive partial ordering, rather than dipole interactions, and hints at a mechanism for ice Ih's transition into ordered ice XI that may extend to other disordered phases. These empirical insights have broader implications for non-periodic systems exhibiting local-symmetry, while enhancing our knowledge of lattice dynamics of this most intriguing material.

Topical Area: Emerging research and multimodal techniques

Poster # - 35

Generating Neutron Orbital Angular Momentum

Sam McKay (Indiana University) David V. Baxter (Indiana University); Kaleb Burrage (Neutron Technologies Division, ORNL); Robert M. Dalgliesh (ISIS Neutron and Muon Source); Fumiaki Funama (Neutron Technologies Division, ORNL); Ivan I. Kravchenko (Center for Nanophase Materials Science, ORNL); Steve Kuhn (Neutron Technologies Division, ORNL); Nickolay V. Lavrik (Center for Nanophase Materials Science, ORNL); Quan Le Thien (Indiana University); Fankang Li (Neutron Technologies Division, ORNL); Gerardo Ortiz (Indiana University); Steven R. Parnell (ISIS Neutron and Muon Source); Roger Pynn (Indiana University)

There is growing interest in the generation of optical and neutron beams with orbital angular momentum (OAM) due to their numerous unique and useful properties [1]. An OAM beam is defined by its phase singularity $e^{i \ell \phi}$ where ℓ is the integer OAM quantum number and ϕ the azimuthal angle defined about the beam's direction of travel.

We present two neutron spin-echo experiments that demonstrate the generation of neutron OAM, one using magnetic Wollaston prisms (MWPs) and the other using a 2D array of forked diffraction gratings (FDGs) etched from a silicon wafer. MWPs generate OAM by using strong magnetic fields and high-temperature superconducting films to ensure sharp transitions between the field regions [2]. In addition to OAM, MWPs in the 2D spin-echo modulated small-angle neutron scattering (SEMSANS) configuration can also produce high-polarization spin textures when properly focused on the detector [3]. We have demonstrated the ability to produce a wide variety of neutron spin textures, and from these textures we can indirectly verify the production of neutron OAM.

On the other hand, FDGs are non-magnetic and can thus be used with techniques such as spin-echo small-angle neutron scattering (SESANS) that require non-depolarizing samples [4]. We demonstrated the production of OAM from FDGs using radio-frequency (rf) neutron spin flippers with SESANS. These experiments show that both MWPs and FDGs can generate high-fidelity states of neutron OAM which may have future application in the measurement of spin-textured and topological materials.

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Topical Area: Emerging research and multimodal techniques

Poster # - 38

Optimizing In situ liquid ToF-SIMS using SALVI and IONTOF M5-NCS

Jiyoung Son (ORNL) Anton Ievlev; Jacob Shusterman (ORNL); Xiao-Ying Yu (ORNL)

In situ time-of-flight secondary ion mass spectroscopy (ToF-SIMS) was enabled to study liquids using a vacuum compatible microfluidics device. This approach has brought a wider range of sample analysis capabilities in vacuum instrumentation, specifically applications in interfaces involving the condense liquid phase. The success operation of in situ ToF-SIMS also has been presented previously using an IONTOF V instrument. We establish in situ liquid ToF-SIMS using the IONTOF MS-NCS instrument at the Oak Ridge National Laboratory (ORNL). Several parameters in the instrument setting (i.e., Primary beam current, voltage, pulse mode) were modified to optimize signal intensity and obtain more effective data collection in a wide mass range. A systematic study was performed including LMIG aperture, tip material of primary gun, primary beam current, voltage, and microfluidic device condition. If just following the procedure for the IONTOF V instrument, in situ liquid SIMS data suffered from low secondary ion intensity and only a narrow mass range was available for spectral and image collection. To acquire higher secondary ion counts, one procedure is not possible to "fit for all" for different ToF-SIMS instruments. In this work, we will present findings of in situ liquid ToF-SIMS optimization using the IONTOF M50NCS platform located in the center for nanophase materials science (CNMS) at ORNL. We demonstrated higher mass resolution in liquid SIMS spectral acquisition using the LIMG buncher voltage mode. Higher total secondary ion counts per sec (~40k ions / sec) with altering single pulse width of the LMIG primary beam was also achieved. The optimized in situ liquid SIMS procedure will be used to study complex interface chemistry in the future.

Topical Area: Emerging research and multimodal techniques

Poster # - 41

Neutron Scattering in High Magnetic Fields: Community Recommendations to Seize the Moment for Scientific Breakthroughs

Matthew Stone (Oak Ridge National Laboratory); Collin Broholm; Despina Louca (University of Virginia); Martin Mourigal (Georgia Institute of Technology); Stuart Calder (ORNL)

Three working groups were formed and led by members of the neutron scattering user community with support from ORNL instrument scientists. The groups examined 1) the science enabled by the largest static magnetic fields, requiring fixed, dedicated installations, 2) the scientific opportunities from static magnetic field sample environments that can be moved between and operated on multiple instruments, and 3) the science enabled by time-dependent and pulsed magnetic field sample environments. The working groups met online during the spring, summer and fall of 2024. This poster describes the series of magnetic field sample environments which were proposed based upon those discussions.

Topical Area: Emerging research and multimodal techniques

Poster # - 45

Localizing Low-Grade Heat Utilizing Infrared Plasmonic Dimers

Gordon Duddy (University of Notre Dame) Jon Camden (University of Notre Dame); Jordan Hachtel (CNMS); David Masiello (University of Washington); Bernadeta Srijanto (CNMS)

Best Student Presentation Award Entry

Plasmonics has profoundly improved our ability to confine light and energy to regions far below the diffraction limit. There is intense recent interest in utilizing infrared-active plasmonic materials to direct infrared energy at the nanoscale and to tailor the material properties via interaction with low-frequency phonons. Furthermore, when resonant in the IR plasmonic structures can couple to substrate phonons and thermally populate localized surface plasmon resonances (LSPRs). While visible plasmons have been extensively studied using electron spectroscopy performed inside a scanning transmission electron microscope (STEM), expanding these studies to the infrared requires a highly monochromated STEM. Using the Nion Hermes 100 MAC-STEM at Oak Ridge National Laboratory, we previously imaged the localization of thermal gain around gold nanorods using electron energy gain spectroscopy (EEGS). More recently, we are performing in-situ heating experiments on more complex systems of nanorod and bowtie dimers. These samples were created with electron beam lithography (EBL), featuring lengths in the micron range and a nanogap of approximately 20 nm. Upon heating to 900°C, we observed thermal population of plasmonic hot spots in the gaps. In this way, diffuse thermal energy was concentrated into an LSPR that could later be coupled with an emitter or other plasmonic structures to extract energy from the system.

Topical Area: Emerging research and multimodal techniques

Poster # - 71

Investigating the Morphology and Optoelectronic Properties of Solution-Processed ITO Multilayer Thin Films using Neutron Scattering and Complimentary Advanced Multimodal Characterization Techniques

Mikis Mays (Georgia Institute of Technology) Rosario Gerhardt

Indium Tin Oxide (ITO), a transparent conducting oxide, is used industrially as an electrode for usage in LEDs, computers/phone screens, and photovoltaic devices. Most ITO thin films are deposited using RF vacuum deposition. An alternative deposition method known as sol-gel deposition, has the benefit of device fabrication under atmospheric conditions and wastes less material than sputtering. However, solution processing methods tend to have higher sheet resistances compared to vacuum-deposited films [1,2] and can suffer from formation of large pores [3]. The spin-coat method was employed to deposit ITO multilayer thin films onto sodium silicate glass substrates. Samples were characterized using a battery of techniques including NR, XRR, ToF-SIMS, TEM and S/STEM.

In this study, we synthesized ITO inks following previously used procedures [4,5] but lowered the relative humidity to 19% during film deposition in hopes of minimizing the formation of voids in the thin film structures. AFM did not reveal any surface pores in contrast to earlier samples. The results of the X-Ray and Neutron scattering length density experiments depicted peaks and troughs located at the interfacial layers of the 1L-5L ITO thin films, respectively. These features are a function of Indium-ion scattering length density being different than that of ITO for both NR and XRR. Additionally, STEM-HAADF images reveal porous ITO layers with increased density at the interfacial regions between layers. EELS was employed, confirming that density rises with increased through-plane depth in the multilayer films. Additionally, EELS revealed increased Indium and Oxygen intensity peaks at the interfacial regions. However, Tin did not experience increased peak intensity at the interface. ToF-SIMS results support EELS data, simultaneously depicting increased Indium-ion content and banded Tin-deficient regions at interfacial layers.

Topical Area: Emerging research and multimodal techniques

Poster # - 72

Analysis of Dark Mirror Neutron Search Experiment

Nathan Whittington (University of Tennessee)

Best Student Presentation Award Entry

Mirror matter has been proposed as a potential explanation for dark matter, with neutron-mirror neutron ($n \leftrightarrow n^{\prime}$) oscillations providing a possible signature of its existence. To search for this effect, we conducted an experiment using a cold neutron beam and the GP-SANS instrument at the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory. The experiment aims to observe these oscillations within a specific dark matter model in which neutrons and mirror neutrons have a slightly different mass (Δm). Under this hypothesis, a magnetic field can compensate for this effect otherwise forbidden by Δm. In our configuration, a cadmium absorber is placed between two 25-Gauss magnets. Ordinary neutrons are blocked by the cadmium, while mirror neutrons—which do not interact with normal matter—pass through, traverse the second magnetic field, and regenerate into detectable neutrons. Given the low probability of oscillation, careful distinction between signal and background was essential. Preliminary analysis yields an effect probability of $(0.11 \pm 2.56) \times 10^{-13}$ per neutron, establishing a limit for probability of this Δm-model to be $< 5 \times 10^{-13}$ per neutron with 95\% confidence. Our further experiments at HFIR will explore alternative models of ($n \leftrightarrow n^{\prime}$) oscillations.

Topical Area: Emerging research and multimodal techniques

Poster # - 95

Investigating Bacterial Behavior on Nanostructured TiO2 to Guide Antifouling Surface Engineering

Parth Desai (North Carolina Agricultural and Technical State University (NCAT)) Shyam Aravamudhan (North Carolina Agricultural and Technical State University); Kristen Dellinger (North Carolina Agricultural and Technical State University); Narendra Lakal; Binod Rizal (North Carolina Agricultural and Technical State University)

Understanding bacterial adhesion on biomaterial surfaces is critical for developing anti-bacterial and/or anti-fouling surfaces. In this study, we investigate two clinically relevant bacterial strains—Escherichia coli ATCC 25922 and Staphylococcus aureus ATCC 49775—on titanium dioxide (TiO_2) nano structured and flat surfaces, and bare glass substrates. Our goal is to elucidate how nanoscale topography of the surface influence bacterial attachment and viability.

We fabricated TiO_2 nanostructures with varying nano-bump densities and interspacing and characterized their surface morphology using atomic force microscopy (AFM). Surface roughness parameters were quantified, and grain density analysis was performed using Gwyddion software. Water contact angle measurements were used to assess surface hydrophobicity and correlate it with bacterial adhesion trends.

To evaluate bacterial attachment, we employed fluorescence microscopy to quantify surface coverage over 24hr and distinguish between live and dead cells. Scanning electron microscopy (SEM) provided high-resolution visualization of bacterial morphology and adhesion patterns across different surfaces. Comparative analysis revealed that nanostructured TiO_2 surfaces significantly altered bacterial adhesion behavior relative to flat titanium and glass, with variations in adhesion energy linked to nano-bump density and wettability.

Our findings suggest that engineered nanoscale features on TiO_2 surfaces can modulate bacterial attachment due to the variation in nanostructure density and spacing on the surface. This work provides a foundation for predictive modeling of surface adhesion energy and offers insights into the design of next-generation antibacterial surfaces.

Topical Area: Emerging research and multimodal techniques

Poster # - 99

CT Scan Visualizer

John Duggan (Oak Ridge National Laboratory) Andrew Ayres (Oak Ridge National Laboratory); Gregory Cage (Oak Ridge National Laboratory); Kenneth Moreland (Oak Ridge National Laboratory); Dave Pugmire (Oak Ridge National Laboratory); Greg Watson (Oak Ridge National Laboratory); Sergey Yakubov (Oak Ridge National Laboratory)

Building upon the Neutron Data Interpretation Platform (NDIP) and the Neutrons Open Visualization and Analysis (NOVA) framework developed at Oak Ridge National Laboratory (ORNL), we have developed a VTK-based interactive software tool, CT Scan Visualizer, for performing rapid visualization of data produced by imaging instruments such as VENUS at the Spallation Neutron Source (SNS). This data commonly takes the form of a stack of 2D Tagged Image File Format (TIFF) images, so the stack represents a 3-dimensional volume. Our tool can take several hundred gigabytes of this type of data and display an interactive volume rendering and slices of the data in a few seconds. While existing tools can provide detailed volume rendering and slicing, this achieves a level of responsiveness and integration with our facilities to open the possibility to perform on-the-fly volume rendering as instruments produce data. The tool allows the user to browse through their experiments and select the data they want to display. It additionally provides controls for swapping between rendering modes and thresholding the data to be visualized. In this talk, we will demonstrate the application, detail how it works, and discuss potential future opportunities.

Topical Area: Emerging research and multimodal techniques

Poster # - 115

High Temperature Stability and Atomic Segregation in Compositionally Complex RE Zirconates Defect-Fluorites

Jade Holliman Jr. (University of Tennessee, Knoxville) Sean Drewry; Katharine Page (University of Tennessee and Oak Ridge National Laboratory); Dante Quirinale (Oak Ridge National Laboratory); Joshua Safin

Compositionally complex oxides (CCOs) are promising candidates for thermal barrier coatings (TBCs) due to their low thermal conductivities, which arise from enhanced phonon scattering caused by cation disorder[1]. Compositionally complex rare-earth (RE) zirconate defect-fluorites ($RE_2Zr_2O_7$) combine low thermal conductivity with high melting temperatures, making them attractive for high-temperature applications. Several $RE_2Zr_2O_7$ compositions were synthesized via solid-state reaction, and preliminary laboratory X-ray diffraction (XRD) confirmed the formation of single-phase defect-fluorite structures. The room-temperature thermal conductivities of equiatomic compositions were measured using the transient plane source (TPS) method. Notably, $(GdDyErYb)_2Zr_2O_7$ exhibited an ultralow thermal conductivity of ~0.9 W/m·K. To investigate the influence of processing on cation ordering, compositions $(TbYb)_2Zr_2O_7$ and $(TbHoYb)_2Zr_2O7$ were synthesized utilizing two milling methods, traditional ball milling and speed-mixing. To better understand the temperature-dependent structural evolution and persistence of atomic segregation, we conducted high-temperature neutron scattering and pair distribution function (PDF) measurements. Using aerodynamic levitation combined with laser heating, we probed the long- and short-range order at elevated temperatures (1200 – ~3,000 °C) relevant to service conditions. The defect-fluorite structure exhibited phase stability above 2,200 °C and recrystallization when cooled from a partial melt. These insights into high-temperature structural behavior will inform future efforts to design next-generation TBCs optimized for extreme environments in energy production, storage, and conversion systems.

1. Yang, Z., et al., Thermal and oxygen transport properties of complex pyrochlore RE2InTaO7 for thermal barrier coating applications. Journal of the European Ceramic Society, 2020. 40(15): p. 6229-6235.

Topical Area: Emerging research and multimodal techniques

Poster # - 118 (Wednesday CNMS Poster Session)

A Fiber-Based NV Center Microscope for Magnetic Field Imaging

Jeremy Trimble (Center for Nanophase Materials Sciences / ORNL)

We present the development of a scanning fiber-based nitrogen-vacancy (NV) center microscope for magnetic imaging under ambient conditions. The system integrates a microdiamond containing a high density of NV centers affixed to the end of an optical fiber, enabling remote excitation and collection of NV fluorescence. The sample is mounted on a 3D nanopositioning stage below the fiber tip, allowing precise scanning across the sample surface. By employing optically detected magnetic resonance (ODMR), the microscope is capable of mapping local magnetic fields with 150 micron resolution. We demonstrate magnetic imaging of battery cathode materials and discuss the system's sensitivity, spatial resolution, and potential for time-domain measurements.

Topical Area: Emerging research and multimodal techniques

Poster # - 34

Probing Thermal Degradation of Li-ion Battery Layered Oxide for NMC 333 Cathodes by Neutron Diffraction

Margarita Petrova; Margarita Petrova Jue Liu (Oak Ridge National Lab); Katharine Page (University of Tennessee and Oak Ridge National Laboratory); Thomas Proffen

Lithium-ion batteries employing $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC333) cathodes face critical safety challenges due to oxygen release and structural collapse at elevated temperatures. This study combines in-situ neutron total scattering (NOMAD beamline, SNS) and operando gas analysis to resolve atomic-scale structural dynamics and gas evolution during thermal degradation (25–550°C). This work aims to determine critical temperatures for layered oxide in NMC 333 cathode material during structure degradation, oxygen gas release, and structural phase transition. Results demonstrate that abnormal change in average bond length for Li-O and Me-O, changes in cell parameters a, c, and cell volume indicate temperatures at which "hidden" phase changes take place. Structural evolution correlates with changes in Ni occupancies at atomic sites, revealing phase transitions. Evolution of oxygen compliments information about temperature ranges with phase transitions. There are additional slope changes in cell parameters as function of temperature not explained with Rietveld analysis results. Beyond long-range order, PDF function provides information about short-range order in local atomic structure and reveals more complex mechanisms for structural evolution. These findings will enable targeted diagnostic metrics for early thermal runaway detection, and targeted suppression of oxygen release via Ni-site stabilization which can aid in design of cathode materials with improved thermal stability.

Topical Area: Hard matter: energy materials

Poster # - 40

Investigating the Influence of Amorphous/Crystalline IrOx on Performance and Degradation Mechanism for Proton Exchange Membrane Electrolyzer Cells (PEMECs)

Jun Li; Weitian Wang; Rebecca Conner; Qi Cai; Ziying (Nancy) Lei; David Cullen; Zili Wu; Feng-Yuan Zhang

Best Student Presentation Award Entry

Hydrogen (H2) with the sustainable and environmentally-benign H2/water cycle has been considered as the candidates for the next-generation clean energy vehicles. PEMECs have advantages of high efficiency, compact design, and near-zero emissions, making it attract unprecedented attention and have been regarded as the more promising water electrolysis technology in the future. Iridium oxides (IrOx) is a leading catalyst for the oxygen evolution reaction (OER) due to its high efficiency and corrosion resistance, However, the mechanisms responsible for its performance loss, dissolution, and degradation, especially those related to structural transition states, are still poorly understood. To investigate this, we used the cutting-edge optical photothermal infrared (O-PTIR) to characterize the structure of the electrodeposited IrOx under various conditions. we focuses on investigating the structural transition from amorphous to crystalline IrOx influence on OER performance and degradation mechanism in PEMECs by using O-PTIR. Our results have demonstrated that the structure of IrOx can transit under different conditions and that the OER performance varies with different IrOx structures: (1) the annealing temperature influences the structure of IrOx, transforming it from amorphous to crystalline as the temperature increases; (2) electrochemical activation induces a structural transition from amorphous to semi-crystalline (partially amorphous, partially crystalline). This work provides new insights into foundational knowledge for IrOx structures for highly efficient PEMECs.

Topical Area: Hard matter: energy materials

Poster # - 42

Average and local structure of ATiO3-δHy (A = Ba, Sr, Ca)

Kennedy Agyekum Bernadette Cladek (University of Tennessee); Jue Liu (Oak Ridge National Lab); Katharine Page (University of Tennessee and Oak Ridge National Laboratory)

Best Student Presentation Award Entry

The reduction of perovskite oxides into oxyhydrides such as ATiO3-δHy (A = Ba, Sr, Ca) affords them unique redox capabilities that enable tunable crystal structure, chemistry, and band gaps, coupled with mixed ionic-electronic conductivity, and new chemical reactivities not present in the parent oxides. These properties make oxyhydrides useful for solid-state hydrogen conductors, hydrogen storage and separation membranes, photocatalysis, anion-engineered electronics, and photochromic applications. The variations in Ti local environment, oxygen vacancy content, and oxygen-oxygen distances, which depend on the A-site cation and hydride concentration, are factors that impact the ionic and electronic transport of ATiO3-xHy. However, fundamental understanding of their defect chemistry, changes in Ti octahedral environment, and controlled hydride incorporation remains limited. In this work, we have employed total scattering techniques to characterize the local and average structures, quantify hydride content and site defects in ATiO3-δHy perovskites. We achieved varied levels of hydride substitution, with up to 18 % hydride incorporation at the anion site. Increasing H content leads to slight cell expansion, reduced oxygen site occupancy, changes in local structure (notably Ti-O, O-O, and A-O pairs), and Ti4+ reduction. The extent of hydride uptake and resulting anion-site defects is sensitive to the A-site cation, enabling direct structural and chemical tuning. These findings provide essential insights for the rational design of perovskite-based hydrogen conductors and related functional materials.

Topical Area: Hard matter: energy materials

Poster # - 46

Flying On The Wings Of Light

Dimitar Dimitrov (Tuskegee University) Elijah Taylor-Harris (Tuskegee University)

Photonic Crystal Light Sails can travel through space without fuel on board and sustain a slight but continuous laser-driven acceleration for an extended period. Numerical simulations have shown that a specific type of Anisotropic Photonic Crystal Slab with three different dielectric constant regions exhibits a complete Photonic Band Gap for a narrow frequency range and is transparent for the rest of the light spectrum. The photonic device consists of small-diameter, high-index-of-refraction Germanium pillars and large-diameter, empty holes, all encapsulated by a low-index-of-refraction polymer. Such a structure has a significantly improved area-to-mass ratio, primarily due to its empty space. Several other advantages over current Light Sails materials have been observed. Initially, a Proof-of-principle sample was manufactured at the Center of Nanophase Material Sciences. Later, two fully functional devices were fabricated, one with equal diameters of pillars and holes, and the other with large holes and small pillars. Currently, the devices are under investigation to measure their spatial, transmission, reflective, and absorptive properties. Later this year, more samples are planned to be manufactured featuring different spatial patterns. The most challenging task is to create a layered three-dimensional photonic crystal, based on he already manufactured slab. Ultimately, the final step is to fly our photonic crystal into space.

Topical Area: Hard matter: energy materials

Poster # - 50

Evaluation of Imbedded Barium in Graphite for Nuclear Engineering in ToF-SIMS

Gabriel Parker (Oak Ridge National Laboratory) Thomas Muth (Oak Ridge National Laboratory); Victor Bautista (Oak Ridge National Laboratory); Xiao-Ying Yu (ORNL)

Advanced manufacturing of cermets, heat-resistant materials made of ceramic and sintered metal, is necessary for radio isotope production to decrease waste and increase efficiency. The High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory currently uses Al as the filler material for irradiation targets. While Al has offered the ease of use and high thermal conductivity, it is limited by the post processing procedures creating a high charge density of the Al cation, creating instable aluminum nitrates, and forming oxidation decreasing the overall performance of the irradiation target. Transitioning from Al to a graphite matrix could reduce the issues aluminum poses. Graphite has similar thermal stability, thermal conductivity, and chemical properties. The manufacturing process using carbon can reduce waste by lowering solution volumes and overall complexity. 223Ra is a radio isotope used for cancer treatments and is produced via a series of beta decays starting with 226Ra. To test method development, Ba, is used as a surrogate to radium. This work examines the barium encapsulation by graphite using time-of-flight secondary ion mass spectrometry (ToF-SIMS). Specifically, high resolution spectroscopy and 2D/3D imaging modes were used to study the BaCO3 pellets prepared in different manner. Current manufacturing process uses a mixture of graphite and barium carbonate either vacuum hot pressed or cold pressed and sintered. The mass spectrometry results verify that BaC as this is the preferred extraction radio isotope and not the oxide or carbonate. Also, depth profiling results show the BaCO3, BaC2, and BaO distributions across the surface and into the bulk of the pellet, indicative of the usefulness of different pellet processing steps.

Topical Area: Hard matter: energy materials

Poster # - 55

Combustion Synthesis of Mn-Rich Disordered Rocksalt (DRX) Oxyfluoride Cathodes for Li-ion Batteries

Max Markuson Diprince (Oak Ridge National Laboratory) Beth Armstrong (Oak Ridge National Laboratory); Ethan Self (Oak Ridge National Laboratory)

Best Student Presentation Award Entry

Lithium-excess disordered rocksalt (DRX) materials are a promising class of Co- and Ni-free lithium-ion battery cathodes that offer high specific energy density (up to 1000 Wh kg^{-1}) and reversible capacity (up to 300 mAh g^{-1}). Compared to traditional Li-ion cathodes (e.g., LiNi$_x$Mn$_y$Co$_{1-x-y}$O$_2$), DRX oxides/oxyfluorides are compatible with a wider range of earth abundant transition metals, such as Ti and Mn. DRX cathodes are traditionally synthesized via solid-state or mechanochemical reactions, which are difficult to scale and provide little control over particle morphology. Furthermore, recent development of DRX compositions show Mn-rich concentrations substantially improve performance by increasing Mn-redox and inhibiting irreversible O-redox. To address this issue, the present study reports a scalable, two-step reaction route to prepare Mn/Ti-based DRX oxyfluoride cathodes with the nominal composition Li$_{1.1}$Mn$_{0.8}$Ti$_{0.1}$O$_{1.9}$F$_{0.1}$ (LMTF1811). The first step utilizes a glycine-nitrate combustion reaction to produce an orthorhombic Mn$_{0.8}$Ti$_{0.1}$O$_{1.4}$ (MTO814) precursor, which is subsequently lithiated and fluorinated by reacting with Li$_2$CO$_3$ and LiF. The effects of annealing temperature (900°C-1100°C) and cooling rate (5-120°C min^{-1}) on the product's structure and DRX phase conversion are explored. Interestingly, heating at 1000°C and quenching between 5 and 120°C min^{-1} shows varying phase purities between 80 and 95%, respectively. However, heating to 1100°C produces Mn-rich phase-pure DRX regardless of quench rate. Phase-pure DRX prepared through this novel synthesis platform exhibit promising electrochemical performance, attaining reversible capacities ~200 mAh g^{-1} with 86% capacity retention after 100 cycles in Li metal half-cells.

Acknowledgements

SEM imaging was performed at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility. Research was conducted at Oak Ridge National Laboratory, managed by UT Battelle, LLC, for the US Department of Energy (DOE) and was sponsored by the Office of Energy Efficiency and Renewable Energy (EERE) in the Vehicle Technologies Office (VTO) through the DRX+ consortium.

Topical Area: Hard matter: energy materials

Poster # - 69

ToF-SIMS Analysis of Coke-Resistant Two-Dimensional Metal Carbide Catalysts

Tobias Misicko (Oak Ridge National Laboratory and Louisiana Tech University) Gabriel Parker (Oak Ridge National Laboratory); Yang Xiao (Louisiana Tech University); Xiao-Ying Yu (ORNL)

Best Student Presentation Award Entry

Catalysts can be described by three important aspects: activity, selectivity, and stability. Activity is the ability of a catalyst to convert reactants into products. Selectivity is the ratio of the desired product to the total amount of converted molecules. Stability is the ability of a catalyst to maintain activity with respect to time on stream (TOS, time since initial contact of reactant gas to the catalyst bed) in continuous reactors. MXene, a class of two-dimensional metal carbides, can be used as a support material to create a coke-resistant nanolayer catalyst with excellent activity, selectivity, and stability. In our prior studies, platinum (Pt) was loaded onto Mo2TiC2 MXene using incipient wetness impregnation to synthesize a 0.5% (wt.) Pt/Mo2TiC2 Pt nanolayer MXene catalyst. The Pt nanolayer catalyst exhibited excellent activity with turnover frequencies (TOFs, converted molecules per surface Pt atom) of 0.4~1.2 s-1 for converting methane and ethane. 0.5% Pt/Mo2TiC2 displayed high selectivity, over 98% to C2 products for non-oxidative coupling of methane(NOCM) and over 95% selectivity for catalytic dehydrogenation of ethane to ethylene. Stability is obtained with no loss in catalytic activity for 72 hr. and 24 hr. TOS for NOCM and ethane dehydrogenation, respectively, owing to strong coke-resistance. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a highly sensitive surface analysis technique capable of molecular, atomic, and isotopic analysis. Coupling ToF-SIMS with sputtering allows for analysis of subsequent monolayers of a sample's surface. Measurements, including surface spectra, mass spectral imaging, secondary electron imaging, and depth profiling, were used to probe the surface and bulk structures of both unloaded Mo2TiC2 MXene support and 0.5% Pt/Mo2TiC2 nanolayer MXene catalysts. The large dispersion of Pt+ ions throughout the bulk of Pt/Mo2TiC2 nanolayer MXene supports the hypothesis that the MXene channel prohibits access to the terrace site, a critical site for the structure-sensitive coking reaction

Topical Area: Hard matter: energy materials

Poster # - 73

Giant Electric-Field Induced Thermal Switching Controlled By Phonon Scattering In A Relaxor Ferroelectric

Puspa Upreti (Oak Ridge National Laboratory) Douglas Abernathy (Oak Ridge National Laboratory); Joseph Heremans (Ohio State University); Raphael Hermann (Oak Ridge National Laboratory); Michael Manley (Oak Ridge National Laboratory); Delaram Rashadfar (Ohio State University); Raffi Sahul (Amphenol Corporation)

The demand for high energy efficiency drives intense interest in thermal management technology. The active control of heat flow in materials can dramatically enhance device efficiency. Lattice vibrations are a major contributor to heat transfer in solids and controlling them through external stimuli is a key challenge for thermal management. However, altering phonons is difficult due to their weak and complicated interactions with external fields. Here, we report significant changes in phonon spectra and transport with the application of an electric field in commercially used relaxor-based ferroelectric PMN-30PT {(1-*x*)[PB(Mg1/3Nb2/3)O3]-xPbTiO3(*x*=30)} using neutron scattering and transport measurements. Phonons sharpen in the direction of the applied poling field and this results in a tripling of the thermal conductivity along the poling direction. We also observe a suppression of nanoscale antiferroelectric fluctuations along the poling direction and argue that this drives the decrease in phonon scattering. This work highlights the potential of relaxor ferroelectrics for realizing solid state heat switching, offering a promising avenue towards high-efficiency thermal management.

Topical Area: Hard matter: energy materials

Poster # - 103

Cu-Based Chalcogenide Nanocrystals $Cu_2ZnA(S_xSe_{4-x})$ (A = Al, Ga, In): Synthesis, Characterization, and S–Se Alloying Effects

Tatiana Allen (Department of Chemistry and Physics, University of Tennessee-Chattanooga); Panchapakesan Ganesh (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Jingsong Huang (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Godwin Mante (Chemical and Materials Engineering, University of Dayton); Soubantika Palchoudhury (Chemical and Materials Engineering, University of Dayton); Prem Shah (Department of Physics, Idaho State University)

We report a new class of Cu-based chalcogenide nanocrystals, $Cu_2ZnAS_xSe_{4-x}$, (A= Al, Ga, In), synthesized via a novel modified hot-injection route. The nanocrystals were experimentally characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-vis absorbance spectroscopy, and steady-state and time-resolved photoluminescence (PL). Analysis of XRD peak intensities showed that all compositions crystallize into pure wurtzite phase (space group: P63mc, no. 186). Scherrer analysis of the peak broadening observed in the diffraction pattern showed nanocrystal sizes ranging from 2.7 ± 0.9 to 11.2 ± 0.8 nm, consistent with TEM imaging. These materials exhibit a direct band gap with strong absorption in the visible range, making them promising candidates for solar spectrum harvesting in photovoltaics. Optical absorption measurements and Tauc plot analyses yielded estimated bandgaps between 2.2 and 3.0 eV. S-Se alloying allows for fine tuning of bandgaps through selenium concentration, with higher selenium content correlating with larger crystallite size and lower bandgap. Theoretical calculations using density functional theory within the virtual crystal approximation also support these observations. PL characterization showed a broad fluorescence spectrum with a peak located in the violet spectral region, around 435 nm (2.85 eV). This energy is close to the estimated direct bandgap value, suggesting emission from direct inter-band transitions. Time-Resolved Photoluminescence (TRPL) showed similar lifetimes across all samples, varying between 2.0 and 2.5 ns, when fitted with a single exponential decay model. The similarity of the TRPL lifetime data suggests a common trapping mechanism that dominated the recombination processes in all the samples, most likely hole trapping. In summary, these new materials exhibit tunable optoelectronic properties, making them promising for photovoltaics and light-harvesting applications requiring absorption in the visible range.

Topical Area: Hard matter: energy materials

Poster # - 4

Modeling The Coupling Between Phonons And Crystal Electric Fields

Allen Scheie (Los Alamos National Laboratory) Caitlin Kengle (Los Alamos National Laboratory); Sabrina Li (Los Alamos National Laboratory); Daniel Rehn (Los Alamos National Laboratory); Wolfgang Simeth (Los Alamos National Laboratory)

Vibronic states are frequently observed in neutron scattering when excited crystal electric field (CEF) levels and phonons are in the same energy range. Typically this coupling is modeled phenomenologically. Here we successfully model the phonon-CEF coupling from first principles using density functional theory and an electrostatic point charge model. We find we are able to account for the observed spectroscopic broadening in several Ce materials, and account for mysterious extra modes found at high energies.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 14

Nanofabrication And Integration Of Quantum Spin Liquid Materials Into Test Structures And Devices.

Ciril Samuel Prasad (CNMS, Oak Ridge National Lab) Sujoy Ghosh (CNMS, Oak Ridge National Lab); Stephen Jesse (CNMS, Oak Ridge National Lab); Debarghya Mallick (MSTD, Oak Ridge National Lab); Steven Randolph (CNMS, Oak Ridge National Lab); Jiaqiang Yan (MSTD, Oak Ridge National Lab)

Best Student Presentation Award Entry

Quantum Spin Liquids (QSLs) emerge in frustrated magnetic materials where spins remain disordered even at 0 K. The presence of quasi-particles, long-range entanglement, and topological order makes QSLs a promising material platform for building inherently fault-tolerant devices for the storage and processing of quantum information. Several recent reports have proposed schemes to test and leverage these unique properties of QSLs, the majority of which involve thermal transport measurements, considering the electrically inactive nature of QSLs. However, realizing such device schemes demands unconventional approaches to nanofabricate and integrate QSL materials into test structures that can reliably operate under cryogenic temperatures (< 2 K) and large magnetic fields (~ 8 T). In this presentation, I will discuss our recent progress in developing a mesoscale thermal transport measurement platform for testing QSLs that can operate under such constraints. I will describe our efforts towards developing ultrasensitive on-chip cryogenic thermal sensors, fabricating suspended nanostructures with minimal thermal leakage, and successfully integrating 2D QSL materials. The development of this platform enables the measurement and control of mesoscale local temperature gradients in QSLs with sub-mK precision, paving the way for further exploration of their fascinating properties and potential applications in quantum technology.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 18

Structural Inhomogeneities and Suppressed Magneto-Structural Coupling in Mn-Substituted $GeCo_2O_4$

Shivani Sharma (Florida State University) Pooja Jain; N. P. Lalla; Benny Schundelmier; Theo Siegrist; Adrienn Maria Szucs; Chin-Wei Wang; Kaya Wei

Best Student Presentation Award Entry

A comprehensive study of $Ge_{1-x}Mn_xCo_2O_4$ (GMCO) system was conducted using neutron powder diffraction (NPD), x-ray diffraction (XRD), Scanning electron microscopy, magnetometry, and heat capacity measurements. Comparative analysis with $GeCo_2O_4$ (GCO) highlights the influence of Mn substitution on the crystal and magnetic structure at low temperature. Surprisingly, phase separation is observed in GMCO with a targeted nominal composition of $Ge_{0.5}Mn_{0.5}Co_2O_4$. SEM/EDX analysis reveals that the sample predominantly consists of a Mn-rich primary phase with approximate stoichiometry $Mn_{0.74}Ge_{0.18}Co_2O_4$, along with a minor Ge-rich secondary phase of composition $Ge_{0.91}Mn_{0.19}Co_2O_4$. Although both GCO and GMCO crystallize in cubic symmetry at room temperature, a substantial difference in low-temperature structural properties has been observed. Magnetic and heat capacity data indicate ferrimagnetic ordering in the Mn-rich phase near TC = 108 K, while the Ge-rich phase exhibits antiferromagnetic order at TN = 22 K in GMCO. Analysis of heat capacity data reveals that the estimated magnetic entropy amounts to only 63% of the theoretical value expected in GMCO. A collinear ferrimagnetic arrangement is observed in the Mn rich phase below the magnetic ordering temperature, characterized by antiparallel spins of the Mn at A site and Co at B site along the c-direction. At 5 K, the refined magnetic moments are 2.31(3) for MnA and 1.82(3) uB for CoB in the Mn rich ferrimagnetic phase. The magnetic structure at 5 K in the Ge rich secondary phase is identical to the antiferromagnetic structure of the parent compound $GeCo_2O_4$. The refined value of the CoB moment in this phase at 5 K is 2.53(3) uB.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 20

Polarized Neutron Triple-Axis Spectrometer (PTAX) For Hard-Condensed Matter Research

Masaaki Matsuda (Oak Ridge National Laboratory) Kaleb Burrage (Oak Ridge National Laboratory); Avishek Maity (Oak Ridge National Laboratory)

Neutron polarization analysis is a powerful technique for condensed matter research. It can separate magnetic and nuclear components, determine the detailed spin direction, and observe weak ferromagnetic component and spin chirality. PTAX/HB-1, installed at the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory, has a variety of polarized equipment, such as Helmholtz coils and cryomagnets, for both elastic and inelastic scattering studies. These studies can be performed in a wide range of temperature (0.05 - 650 K), high pressure ($\leq$ 1.8 GPa), magnetic field ($\leq$ 8 T), and electric field ($\leq$ 10 kV). We have also implemented unique capabilities: the Wollaston Prisms for Larmor diffraction (ultrahigh Q resolution) and inelastic spin-echo (ultrahigh energy resolution) measurements and the Spherical Neutron Polarimetry (SNP) device for studying complex magnetic structures. We will present the instrument capabilities, upgrade plans, and scientific output from the instrument.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 26

Development of the Multi-Analyzer Neutron Triple Axis (MANTA) Spectrometer at ORNL

Adam Aczel (Oak Ridge National Laboratory); Violet Freudenberg (ORNL); Garrett Granroth (Oak Ridge National Laboratory); Mark Lumsden; Martin Mourigal (Georgia Institute of Technology); Gregory Warren (ORNL)

The Multi-Analyzer Neutron Triple Axis (MANTA) Spectrometer is a cold neutron instrument currently in development as part of the planned upgrade to the cold guide hall at the High Flux Isotope Reactor (HFIR). MANTA will replace the current CTAX instrument at HFIR and will boast a factor of 50x improvement in the neutron flux, thereby establishing it as a world-class cold-neutron spectroscopy instrument. This will be achieved by positioning the instrument at the ideal location in a re-optimized cold guide hall and by using modern guides with the geometry and m-coatings established by rigorous McStas simulations. The upgraded incident beamline will also include a neutron velocity selector, virtual source, double-focusing pyrolytic graphite monochromator, modern sample table, and a V-cavity to facilitate incident beam polarization. The design is optimized to provide the maximum flux on a 2cm x 2cm sample with an incident energy between 2.6 and 20 meV. To provide overlap with the thermal instruments, it will operate at higher energies. Phase I of the project will deliver an updated single analyzer-detector backend capable of polarization analysis and a dedicated >=14 T vertical field cryomagnet. Phase II of the project will introduce an interchangeable multiplexed secondary spectrometer based on the IRIS or CAMEA concept. This talk will describe the current status of the MANTA project with a focus on the ongoing pre-conceptual design work for Phase I and some discussion of our plans for Phase II.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 33

Density-Controlled Ion Transport in Amorphous Hafnium Oxide

Dongjae Shin (University of Michigan) Anton Ievlev; Yiyang Li (University of Michigan)

Best Student Presentation Award Entry

Ion conduction in ceramic materials is crucial for the performance and reliability of various functional materials, such as gate dielectrics, electrochemical transistors, and memristors. In crystalline materials, ion conduction depends on point defects like vacancies and interstitials, making ionic conductivity directly proportional to defect concentration and mobility. However, in amorphous materials, such crystallographic point defects are undefined. Our study utilized time-of-flight secondary ion mass spectroscopy (ToF-SIMS) depth profiling to measure oxygen tracer diffusion in amorphous hafnium oxide thin films and found that sub-stoichiometric hafnium oxide (HfO$_{1.74}$) exhibits diffusivity two orders of magnitude lower than stoichiometric hafnium oxide (HfO$_{2}$). Furthermore, among stoichiometric amorphous hafnium oxide thin films, higher-density hafnium oxide film (9.9 g cm^{-3}) demonstrate lower diffusivity compared to their lower-density counterpart (6.8 g cm^{-3}). This finding indicates that traditional defect chemistry fails to describe diffusion trends in amorphous hafnium oxides. Instead, free volume and film density significantly influence oxygen diffusivity. This work underscores that density and free volume are critical design considerations for ionic conduction in amorphous materials, with implications for designing ionic conductors in various applications, including memory devices, and synaptic transistors.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 48

A Panoramic View of MXenes via an Atomic Coordination-Based Design Strategy

Zhongfang Chen (Department of Chemistry, University of Puerto Rico, Rio Piedras); Oyshee Chowdhury (Department of Aerospace Engineering and Mechanics, The University of Alabama); Traian Dumitrica (Department of Mechanical Engineering, University of Minnesota Twin Cities); Panchapakesan Ganesh (Center of Nanophase Materials Sciences, Oak Ridge National Laboratory); Yury Gogotsi (Department of Materials Science and Engineering, and A.J. Drexel Nanomaterials Institute, Drexel University); Chongze Hu (Department of Aerospace Engineering and Mechanics, The University of Alabama); Jingsong Huang (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Jacek Jakowski (Computational Sciences and Engineering Division, Oak Ridge National Laboratory); Paul R. C. Kent (Computational Sciences and Engineering Division, Oak Ridge National Laboratory); Vincent Meunier (Department of Engineering Science and Mechanics, The Pennsylvania State University); Michael Naguib (Department of Physics and Engineering Physics, Tulane University); Noah Oyeniran (Department of Aerospace Engineering and Mechanics, The University of Alabama,); Bobby G. Sumpter (Center of Nanophase Materials Sciences, Oak Ridge National Laboratory); Raymond Unocic (Department of Materials Science and Engineering, North Carolina State University)

Two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, possess unique physical and chemical properties, enabling diverse applications in fields ranging from energy storage to communication, catalysis, sensing, healthcare, and beyond. Despite extensive research and notable advancements, a fundamental understanding of MXenes' phase diversity and its connection to their hierarchical precursors, including the intermediate MAX phases and the ancestral bulk phases, remains limited. Here, we hypothesize that the atomic coordination environments adopted by transition metal and nonmetallic atoms in their 3D bulk precursors may persist in 2D MXenes to govern their phase diversity. Using high-throughput modeling based on first-principles density functional theory, we unveil a wide range of MXene phases and comprehensively evaluate their relative stabilities across a large chemical space. The key to our approach lies in considering various atomic coordination environments drawn from four types of ancestral bulk phases. Through this comprehensive structural library of MXenes, we uncover general guiding principles, such as a close alignment between the phase stability of MXenes and that of their 3D precursors. We further observe that variations in atomic coordination also influence mechanical properties such as stiffness and elasticity, highlighting the broader impact of coordination environments on MXene functionalities. These findings introduce a new design strategy in which the atomic coordination environments in bulk phases can serve as reliable predictors for accessing a broadened landscape of MXenes.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 49

First-Principles Calculations Of Noncollinear Magnetization Densities In Quantum Materials

John Villanova (Middle Tennessee State University) Colin Sarkis (Oak Ridge National Laboratory); Casey Eichstaedt (National Renewable Energy Laboratory); Adolfo Eguiluz (University of Tennessee Knoxville); Stephen Nagler (University of Tennessee Knoxville); Tom Berlijn (Oak Ridge National Laboratory)

Neutron scattering is an established workhorse for detecting signatures of quantum spin liquids (QSLs) including fractionalized excitations. However, this depends on having accurate magnetic form factors to analyze signals. These are commonly treated in an isolated, isotropic ion approximation, but the local magnetic degrees of freedom in QSL candidate materials are j_{eff}=$\frac{1}{2}$ moments which are anisotropic [1] and hybridize with nearby anions. We have developed a Wannier function-based method to simulate both the spin and orbital contributions to the magnetic interaction vector. We show that the associated real-space magnetization densities exhibit intra-atomic noncollinearity. These facets will notably affect neutron scattering measurements and advance beyond the basic magnetic form factor. Using α-RuCl$_3$ as an example, we identify specific scattering directions for neutron experiments to optimally detect the unique quality of the noncollinear magnetization density.

[1] Colin L. Sarkis et al, Phys. Rev. B 109, 104432 (2024).

Acknowledgment: This work is supported by the U.S. Department of Energy, Office of Science, under grant award number DE-SC0025748.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 52

Focused Helium Ion Beam for Direct Patterning of Monolayer MoS2 Nanoribbon Field Effect Devices

Zhihong Chen (Purdue University); Xiangkai Liu (Purdue University); Steven Randolph (CNMS, Oak Ridge National Lab) Joerg Appenzeller (Purdue University); Thomas Beechem (Purdue University); Sujoy Ghosh (CNMS, Oak Ridge National Lab); John Lasseter (ORNL); Sahej Sharma (Purdue University); Dmitry Zemlyanov (Purdue University)

Best Student Presentation Award Entry

Helium focused ion beam (FIB) has emerged as a powerful technique to directly pattern nanostructures below 10 nm due to its high-resolution capabilities, the inert nature of the helium ion source, and high penetration depths as compared to heavier ion sources. These attributes make He FIB particularly interesting for patterning two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) to investigate transport phenomena at ultra-scaled dimensions. We demonstrate the effective use of helium ion microscope (HIM) FIB for fabricating MoS2 nanoribbon array devices, enabled by a volatile XeF2 precursor for gas-assisted FIB-induced etching (FIBIE), which allows for reduced ion dose compared to direct sputtering. While excellent pattern definition is achieved, the resulting devices exhibit significant performance degradation with decreasing nanoribbon width. This is attributed to delocalized damage extending up to 150 nm beyond the patterned edge. Incorporating a thin top encapsulation layer of hBN is found to improve device performance by one order of magnitude, although the lateral extent of damage remains unchanged. These findings suggest that the spatial distribution of damage is primarily determined by the forward- and back-scattered ions and electrons trajectories. The use of the hBN encapsulation layer is found to substantially reduce the damage from XeF2-related processes in unexposed regions. Raman and photoluminescence (PL) measurements corroborate these findings, while ion/solid interaction simulations further elucidate the resolution limits imposed by substrate interactions. This work provides critical insights and a practical pathway for utilizing HIM FIBIE in 2D TMD functional device patterning.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 54 (Wednesday CNMS Poster Session)

High-Throughput, Multi-Scale Modeling of Bi2Se3 Topological Materials

Ryan Morelock (Oak Ridge National Lab) Soumendu Bagchi (Oak Ridge National Laboratory); Panchapakesan Ganesh (Oak Ridge National Laboratory)

This talk presents our progress in developing autonomous workflows that generate DFT data and fit both reactive and machine-learned force fields to guide the molecular beam epitaxial synthesis and characterization of the van der Waals–layered topological insulator Bi_2Se_3. I will introduce pyRMG, our Python package for high-throughput real-space multigrid (RMG) DFT calculations on Frontier, and show how it can be used to explore the potential-energy surface and electronic structures of Bi_2Se_3 films with variable twist angles on $NbSe_2$ superconductor substrates. Next, I'll describe our fitting approaches for ReaxFF and ML (MACE) force fields for the Bi-Se system, and how we've applied Bayesian optimization to navigate the complex MD parameter space for targeted synthesis (e.g., recrystallization pathways). Finally, I'll outline future directions for extending these highly-integrated computational methods to other low-dimensional topological materials and compositional systems.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 59

Tuning the Memristive Behavior in Single-Crystal Transition Metal Dichalcogenides

Dakotah Kirk (Auburn University); Marcelo Kuroda (Auburn University)

Best Student Presentation Award Entry

Memristors based on two-dimensional transition metal dichalcogenides (TMDs) are emerging as key components for future memory and neuromorphic computing technologies. In single-crystal TMDs such as $MoSe_2$ and WSe_2, we attributed that memristive switching to an electrode-facilitated 1H to 1T′ phase transition, stabilized by defect binding [1]. Expanding on this, we present a data-driven framework for the rational design of TMD memristors through interface engineering. Using high-throughput calculations within the density functional theory (DFT) and utilizing machine learning regression models, we systematically investigate how different transition metal electrodes affect the stability of the 1T′ phase across a range of group-VI TMDs (MoS_2, WS_2, $MoSe_2$, WSe_2, $MoTe_2$). We analyze means to control phase stability such as the dielectric environment, electrode defect energetics, and TMD thickness. Our results reveal that electrodes from groups 10–12 (e.g., Cu, Ag, Zn) may improve the memristive performance of the TMDs, as they both decrease phase energy barriers and favor the 1T' phase upon absorption. Additionally, we find that due to the low energy difference between 1H and 1T' phases in $MoTe_2$, bilayer or thicker systems are required to achieve stable switching behavior. These structure-property relationships assist the selection of optimal electrode/TMD combinations and offer valuable design principles to guide experimental development of tunable, high-performance TMD-based memristors. This work is supported by NSF Grant No. 1848344 and is part of a user project at the CNMS.

[1] Kirk et al., ACS Appl. Mater. Interfaces, 17, 23, 34717 (2025).

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 60

Modeling Quantum Materials With Disorder And Interactions In And Out Of Equilibrium

Anirudha Mirmira (Middle Tennessee State University) Eric Dohner (Dept of Physics, University at Albany); Hanna Terletska (Middle Tennessee State University)

Realistic modeling of quantum materials with both interactions and disorder, while challenging, has been a fruitful endeavour in explaining and informing experiments in condensed matter physics. Disorder is not only ubiquitous, but has been shown to give rise to novel phenomena like localization, suppressed critical temperature and metal-insulator transition. Experimental investigations, which almost always deal with non-equilibrium conditions, necessitates a method capable of handling time-dependent systems. Recently, we have developed the DMFT-CPA quantum embedding framework, applicable to both systems in and out of equilibrium, which integrates dynamical mean field theory (DMFT) with the coherent potential approximation (CPA), and systematically probed the physics of the Anderson-Hubbard model subjected to various interaction quench protocols. Particular emphasis is placed on the influence of different disorder distributions, including box, binary, and Gaussian types. In equilibrium, it is seen that the types of disorder considered have qualitatively different effects on the phases, in particular, the binary disorder giving rise to a band insulating phase. Out of equilibrium, we compute the time evolution of single-particle distribution functions and the dynamics of energy following the quench, elucidating the role of disorder in shaping the relaxation pathways and thermalization behavior in strongly correlated, disordered quantum systems. We see that the different disorder types do not show any qualitative differences in the energy and occupation dynamics even in the large binary disorder case, where the equilibrium phase is a band insulator.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 61

Gold Thiolate Coordination Polymers as Potential Phase Change Materials for Data Storage

Meenu Murali (Postdoctoral Research Associate, Department of Chemistry , Washington University in St. Louis) Kelly M Powderly (Department of Chemistry, Washington University in St. Louis)

Coordination polymers (CPs) are emerging functional inorganic-organic hybrid materials formed by the coordination bond between a metal ion or cluster and an organic linker. Phase Change Materials (PCMs) can undergo reversible transitions between an amorphous phase to one or more crystalline polymorphs through external heating. CP-PCMs, with distinct optical and electrical properties that depend on the structure of each polymorph, are proposed as data-storage materials.¹

Recently, Au(I)-thiolate CPs have emerged as a substitute for inorganic PCMs in data storage applications due to their low operating temperature (< 200°C) and flexibility.² These Au(I)-thiolate CPs exhibit an amorphous-to-crystalline and subsequent polymorphic phase transition with increasing temperature. With gentle grinding, the amorphous phase is recovered.² The difference in the photoluminescence of each phase is proposed as an optical signal to store data. To the best of our knowledge, Au(I)-thiolate PCMs with a dithiol molecule as the bridging ligand have not been reported yet.^{2,3}

We report the synthesis of a novel Au(I)-thiolate CP incorporating both biphenyl-4,4′-dithiol (BDT) and 4-methylbenzenethiol (MBT) molecules as bridging ligands. We are studying its reversible tranformations from amorphous to various crystalline phases, focusing on the change in luminescence and electrical properties. For comparison, we have also synthesized the end-member Au(I)-thiolate CPs with a single linker, either BDT or MBT. Detailed investigation of phase transitions and resultant changes in photoluminescence and conductivity in these dithiol-based Au(I)-thiolate CPs will expand the class of CP-PCMs as potential materials for next-generation data storage devices.

Reference

(1) Zou, R et al., *Adv. Mater*. **2022**, *34* (41), 2202457.

(2) Demessence, A et al., *Angew. Chem*. Int. Ed. **2022**, *61* (14), e202117261.

(3) Demessence, A et al., *ACS Appl. Mater. Interfaces* **2024**, *16* (17), 22512–22521.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 62 (Wednesday CNMS Poster Session)

Pulsed Laser Deposition With In Situ Diagnostics: Roadmap To 2D Materials Processing And Synthesis

Gerd Duscher2 (University of Tennessee); David B. Geohegan (University of Tennessee); Sumner B. Harris (Oak Ridge National Laboratory); Austin Houston (University of Tennessee); Alexander Puretzky (Oak Ridge National Laboratory); Ivan Vlassiouk (Oak Ridge National Laboratory); Kai Xiao (Oak Ridge National Laboratory); Daniel Yimam (Oak Ridge National Laboratory)

2D monolayers and heterostructures have become central to nanoscience in recent years, offering promising applications in electronics, sensing, and future computing. Significant progress has been made in 2D materials bottom-up synthesis and subsequent processing, driven by the need for harnessing and exploring exciting functional properties. Techniques such as encapsulation, doping, and implantation in atomically thin 2D materials are crucial to transitioning them from fundamental research to scalable, real-world applications, while also enabling the emergence of novel properties. However, the ultrathin nature that makes 2D materials attractive also poses substantial challenges for traditional plasma-based processing methods. To fully harness the potential, it is essential to develop reliable processing techniques that offer precise control and reproducibility. Pulsed laser deposition (PLD) emerges as a promising non-equilibrium method that allows precise control over the kinetic energy (KE) of ablated species. In our work, we investigate plasma plume interactions with 2D materials using in situ plasma diagnostics and optical characterization tools. Our approach enables low temperature substitution and implantation of foreign atoms, such as chalcogens and metals, facilitating the selective synthesis of Janus monolayers and alloys. We demonstrate that a deep understanding and control of plasma plume dynamics enables new approaches for 2D material engineering, including the formation of Janus monolayers, metal atom implantation, and encapsulation with minimal damage. These findings highlight the potential of PLD to drive the practical advancements in 2D materials for microelectronics and quantum information science.

This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 63

Spin Density Wave Phase Protected By Long-Range Charge Order In A Kagome Antiferromagnet

Feng Ye (Neutron Scattering Division, ORNL) Tingjun Zhang (Rice University)

The interplay between charge density wave (CDW) and spin density wave (SDW) orders in quantum materials play a crucial role in the determination of their electronic, structural, and magnetic properties. Kagome lattice materials provide a platform to study these complex interactions, owing to their exotic electronic structures, including Dirac cones, van Hove singularities, and flat bands. The Kagome metal FeGe (B35 phase) undergoes a sequence of phase transitions upon cooling: it first develops an A-type antiferromagnetic (AFM) order, followed by a $2\times2\times2$ CDW order, and ultimately an incommensurate (IC) SDW order with a propagation vector along the c-axis. Remarkably, the CDW can be tuned—from long-range order to complete suppression—via post-growth annealing, and the onset temperature and ordered moment of the SDW phase exhibit a correlated trend. In this work, we identify FeGe with long-range charge order as a rare example in which the magnetic structure of the SDW phase has been unambiguously determined via neutron diffraction. The magnetic moment of the transverse SDW order exhibits a sinusoidal modulation with an amplitude of 0.94 μB, and the evolution of magnetic domain volume quantitatively accounts for the variation in IC diffraction peak intensities. The observed changes in the incommensurate propagation vector further highlight the coupling between CDW and SDW orders. Polarized neutron diffraction results are also consistent with this magnetic structure model. Moreover, we find that the long-range CDW-modulated lattice stabilizes the SDW order. On the contrary, in samples exhibiting only short-range CDW order, the reported phase transitions between double-cone structures and suppression of ordered moment size are a consequence of the interplay between the magnetic field and imperfect Fermi surface nesting. These findings provide compelling evidence for the itinerant nature of the IC magnetic order and highlight the intricate coupling among lattice, spin, and charge degrees of freedom.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 66

First-Principles Investigation of Ionic Contributions to the Frequency-Dependent Dielectric Function in Cs_2HfCl_6, Cs_2ZrCl_6, and $Cs_2Hf_{0.5}Zr_{0.5}Cl_6$

Elijah Adedeji (Alabama A&M University) Stephen Babalola (Alabama A&M University); Jingsong Huang (Oak Ridge National Laboratory); Eva Zarkadoula (Oak Ridge National Laboratory)

We present a first-principles investigation of the frequency-dependent dielectric properties of halide double perovskites Cs_2HfCl_6 (CHC), Cs_2ZrCl_6 (CZC), and the mixed alloy $Cs_2Hf_{0.5}Zr_{0.5}Cl_6$ (CHZC). Using density functional theory (DFT) and density functional perturbation theory (DFPT), we evaluated both the electronic ($\varepsilon\infty$) and ionic (ε_ionic) contributions to the dielectric response. While $\varepsilon\infty$ remains relatively consistent across all compositions—indicating similar electronic polarizability—ε_ionic increases from CHC to CZC, due to the more polarizable nature of Zr–Cl bonds compared to Hf–Cl. CHZC exhibits intermediate dielectric behavior, suggesting a smooth compositional transition in lattice polarizability.

Phonon dispersion calculations were performed to confirm the dynamic stability of the materials. Lattice parameters and electronic band structures were calculated within the GGA-PBE functional. Preliminary work is underway to estimate the exciton–phonon coupling strength using the Huang-Rhys factor, while planned GW and GW+BSE simulations aim to provide more accurate exciton binding energies and resolve absorption edge characteristics across the alloy series.

These findings highlight the critical role of ionic lattice dynamics and cation substitution in tuning the dielectric and optical responses, with direct implications for enhancing light yield, scintillation decay characteristics, and energy resolution in radiation detection technologies.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 67

Quantum Cluster Embedding Study of Disordered and Strongly Correlated Systems

Hanna Terletska (Middle Tennessee State University) Anirudha Mirmira; Emanuel Gull; Thomas Maier

Quantum materials with strong electronic correlations lie at the heart of modern condensed matter physics, exhibiting rich phenomena such as unconventional superconductivity, Mott insulating behavior, and quantum criticality. Realistic modeling of these systems necessitates the inclusion of disorder, which plays a crucial role in driving metal-insulator transitions (MITs), inducing electron localization, and profoundly impacting transport, spectral, and thermodynamic properties. In this study, we employ quantum cluster embedding techniques within the framework of Dynamical Mean Field Theory (DMFT)—specifically, the Dynamical Cluster Approximation (DCA), Cellular DMFT (CDMFT), and the Typical Medium DCA (TMDCA)—to investigate the interplay of strong correlations and disorder in both two- and three-dimensional Anderson and Hubbard models. Our results reveal significant non-local correlation effects near the localization transition, highlighting the limitations of purely local theories in capturing the full complexity of disorder-driven and interaction-driven MITs. Through a comparative analysis of the different quantum cluster approaches, we benchmark their accuracy and efficacy in resolving key features of the phase transitions. This work demonstrates the essential role of non-local quantum embedding methods in understanding disordered, strongly correlated systems and provides insights into the mechanisms governing the emergence of insulating and metallic phases.

Acknowledgement: This work is supported by the U.S. Department of Energy, Office of Science, under award number DE-SC0025748 grant.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 68

From Flat to Curved: Substrate Morphology as a Design Tool for Magnetic Thin Films

Asmaa Qdemat (SNS)

Topography and curvature at the nanoscale offer unique opportunities to tailor magnetic properties in thin film systems, relevant for future spintronic and neuromorphic applications. In this work, we investigate how substrate morphology introduced via self-assembled SiO_2 nanospheres affects the magnetic behavior of Fe_3O_4 and CoPd alloy thin films, compared to their counterparts grown on flat substrates.

For Fe_3O_4, STEM and GISANS confirm conformal growth with preserved lateral order, while XMCD-PEEM imaging reveals in-plane magnetic domains that span both curved and flat regions. Despite reduced net magnetization in the curved regions, domain alignment across interfaces indicates strong magnetic coupling between structurally distinct areas.

In CoPd thin films, curvature significantly enhances magnetic properties. Polarized neutron reflectometry shows that thinner curved films exhibit higher magnetic scattering length density than thicker ones. SQUID magnetometry reveals increased coercivity and modified anisotropy, while GISANS confirms structural ordering without lateral magnetic coherence, likely due to perpendicular anisotropy or domain averaging.

Together, these results demonstrate that nanoscale topography and curvature can be leveraged to modulate magnetism in both oxide and metallic thin films. This highlights a promising strategy for engineering domain textures and magnetic anisotropy through substrate design, offering pathways toward flexible and high-performance spintronic architectures.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 70

Vibration Spectroscopy and Nanodiffraction of Multi-phase Boron Nitride Thin Films.

Nooreen Qureshi (University of Virginia) Kory Burns (University of Virginia)

Best Student Presentation Award Entry

Epitaxial growth of cubic boron nitride (c-BN) thin films on diamond is a holy grail for high-power electronics as it can efficiently dissipate heat due to its high thermal conductivity. Therefore, extensive efforts are ongoing to grow epitaxial c-BN thin films on diamonds with an atomically smooth interface. Over the course of this study, the early-stage epitaxial growth of few-layer c-BN films on nitrogen functionalized (001) single crystal diamond surface was observed with atomic-scale interpretation. Specifically, the existence of these layers was verified with advanced transmission electron microscopy (TEM) methods, highlighted by monochromated electron energy loss spectroscopy (EELS) to probe phonon transport at strain-driven interfaces and scanning nanodiffraction 4D scanning TEM (4D-STEM) to measure impurity scattering at a localized scale. Ultimately, this work presents a new materials platform for potential applications in next-generation quantum sensors for pressure water reactors, owing to its isotropic thermal properties and supreme radiation hardness.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 81 (Wednesday CNMS Poster Session)

Probing Spin Defects via Single Spin Relaxometry

Alex Melendez (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory) Ruotian Gong (Department of Physics, Washington University in St. Louis); Guanghui He (Department of Physics, Washington University in St. Louis); Yan Wang (Computational Sciences and Engineering Division, Oak Ridge National Laboratory); Yueh-Chun Wu (Materials Science and Technology Division, Oak Ridge National Laboratory); Thomas Poirier (Tim Taylor Department of Chemical Engineering, Kansas State University); Steven Randolph (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Sujoy Ghosh (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Liangbo Liang (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Stephen Jesse (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); An-Ping Li (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Joshua Damron (Chemical Sciences Division, Oak Ridge National Laboratory); Benjamin Lawrie (Materials Science and Technology Division, Oak Ridge National Laboratory); James Edgar (Tim Taylor Department of Chemical Engineering, Kansas State University); Ivan Vlassiouk (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Chong Zu (Department of Physics, Washington University in St. Louis); Huan Zhao (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory)

Spin defects in solid-state systems are powerful platforms for quantum sensing and quantum information storage due to their long coherence times and compatibility with scalable architectures. In this work, we present scanning probe microscopy utilizing the nitrogen vacancy (NV) center in diamond to locally detect and image spin-based quantum sensors at the nanoscale. Specifically, we study the negatively charged boron vacancy (V$_\text{B}^-$) center in hexagonal boron nitride (hBN), itself a promising two-dimensional quantum sensing platform. Rather than relying on the V$_\text{B}^-$ center optical properties, we detect its spin transitions through their impact on the longitudinal spin relaxation time (T_1) of a nearby NV. Relying on cross-relaxation between NV and V$_\text{B}^-$ spins, this indirect detection scheme circumvents the need for optical excitation or fluorescence collection from the hBN itself. When the NV and V$_\text{B}^-$ spin transitions become resonant, the T_1 of the NV shortens significantly, allowing selective sensing of the local V$_\text{B}^-$ density. We use this mechanism to spatially map the distribution of V$_\text{B}^-$ centers with nanoscale resolution, well beyond the diffraction limit of optical imaging. In isotopically purified h^{10}B^{15}N, we further resolve hyperfine interactions, highlighting the sensitivity of the technique to fine spectral features. Our results showcase a hybrid sensing architecture in which 3D NV sensors serve as readout channels for 2D spin systems, opening new possibilities for characterization of optically inactive spin defects in layered materials.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 83

Constraints on magnetism and correlations in RuO$_2$ from inelastic neutron/x-ray scattering and Mössbauer spectroscopy

George Yumnam (Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge) Parul Raghuvanshi (Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge); John Budai (Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge); Lars Bocklage (The Hamburg Centre for Ultrafast Imaging CUI, Hamburg and Deutsches Elektronen-Synchrotron DESY, Hamburg); Douglas Abernathy (Oak Ridge National Laboratory); Yongqiang Cheng; Ayman Said (Advanced Photon Source, Argonne National Laboratory, Lemont); Igor Mazin (Department of Physics and Astronomy, George Mason University, Fairfax, Virginia); Haidong Zhou (Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee); Benjamin Frandsen (Department of Physics and Astronomy, Brigham Young University, Provo, Utah); Lucas Lindsay (Oak Ridge National Laboratory); Valentino Cooper; Michael Manley (Oak Ridge National Laboratory); Raphael Hermann (ORNL)

We provide experimental evidence for the absence of a magnetic moment in bulk RuO$_2$, a candidate altermagnetic material, by using a combination of inelastic neutron and X-ray scattering, Mössbauer spectroscopy, nuclear forward scattering, and density functional theory calculations. The lattice dynamics from our inelastic neutron/x-ray scattering experiments were compared to density functional theory calculated lattice dynamics with various functionals by estimating the dynamic structure factor and the bose-factor corrected dynamic susceptibility. This comparison reveals that the DFT calculated non-magnetic RuO$_2$ structure provides the best description of our inelastic scattering experiments. Using complementary Mössbauer and nuclear forward scattering we also determine the ^{99}Ru magnetic hyperfine splitting to be negligible, which further substantiates the non-magnetic behavior of RuO$_2$. Our comprehensive analysis indicates that the electronic correlations, rather than magnetic order, are key in describing the lattice dynamics.

Acknowledgement: Research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division (BES-MSED). A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. The beam time was allocated to ARCS on proposal number IPTS-17267.1. A portion of this research used resources at the Advanced Photon Source, a DOE Office of Science User Facility operated by Argonne National Laboratory.

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Yumnam, G., Raghuvanshi, P.R., Budai, J.D., Bansal, D., Bocklage, L., Abernathy, D., Cheng, Y., Said, A., Mazin, I.I., Zhou, H., Frandsen, B.A., et al. Constraints on magnetism and correlations in RuO$_2$ from lattice dynamics and Mössbauer spectroscopy, arXiv:2505.03250 (2025).

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 86

Neutron scattering investigation of Tb^{3+} crystal fields in magnetoelastic TbSi

Sierra Diller (Georgia Tech) George Yumnam (Oak Ridge National Laboratory); Ajay Kumar (Ames National Laboratory, Iowa State University, Ames, Iowa); Yaroslav Mudryk (Ames National Laboratory, Iowa State University, Ames); Douglas Abernathy (Oak Ridge National Laboratory); Qiang Zhang (ORNL); Raphael Hermann (ORNL)

Best Student Presentation Award Entry

TbSi is an FeB-type compound exhibiting complex antiferromagnetic behavior with two first-order and one second-order phase transitions. Below 35 K, it exhibits a planar AFM structure then transitions into an incommensurate phase between 35 and 39 K before becoming commensurate again up to the Néel temperature, T_N = 57 K[1]. We measured the temperature-dependent crystal field softening, which is associated with the magnetic structure transition via powder inelastic neutron scattering measurements at ARCS, SNS. The polycrystalline averaged crystal field transitions from a gapped dispersion-like feature at T = 10 K to a smooth ungapped feature at T = 37 K, and paramagnet-like feature above 50 K. Magnetization measurements and heat capacity studies have shown a unique hysteresis of the magnetic transition[2], and we investigated the magnetic structure transitions via quasi-continuous heating neutron powder diffraction from T = 34 to 40 K at POWGEN, SNS.

Research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division (BES-MSED). This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI) (S.D.). A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. The beam time was allocated at ARCS and POWGEN on proposal numbers IPTS-33695 and ITPS-33763, respectively.

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Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 91

Probing the Nanoscale Excitonic Landscape and Quantum Confinement in Gated Monolayer WS2 via Cathodoluminescence

Yueh-Chun Wu; Benjamin Lawrie (Materials Science and Technology Division, Oak Ridge National Laboratory); Bogdan Dryzhakov (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory); Jun Yan (University of Massachusetts Amherst); Kyle Kelley (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory)

Engineering excitonic properties at the nanoscale is a central challenge in quantum photonics and optoelectronics. While far-field optical spectroscopy has greatly advanced our understanding of excitonic phenomena, its diffraction-limited resolution yields only spatially averaged information. In this work, we investigate the excitonic landscape of monolayer WS2 under electrostatic gating using cathodoluminescence (CL) spectroscopy. By leveraging the high spatial resolution of CL, we reveal a locally modulated Stark shift in exciton emission at homojunctions formed between regions with different stacking configurations. Moreover, under electron-beam excitation, we observe a gate-dependent switching of trion species, attributed to beam-induced charge trapping in the hBN dielectric. This unconventional electrostatic doping mechanism enables the formation of an exciton confinement potential, giving rise to a localized exciton channel that can be directly visualized through CL nanoscopy. Our findings elucidate the optoelectronic behavior of monolayer semiconductors under combined e-beam excitation and electrostatic gating. This approach provides a route for nanoscale exciton manipulation and opens opportunities for the control of quantum confined exciton transport in two-dimensional materials.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 93

Epitaxial Strain-Mediated Control of Oxygen Vacancies in SrRuO3 for Enhanced Thermoelectric Properties

Mohammad El Loubani (University of South Carolina) Sepideh Akhbarifar (The Catholic University of America); Scott Bender (University of Virginia); Md Shafkat Bin Hoque (University of Virginia); Patrick Hopkins (University of Virginia); Dongkyu Lee (University of South Carolina); Benjamin Richardson (University of South Carolina); Christopher Rouleau (Oak Ridge National Laboratory); Ebenezer Seesi (University of South Carolina)

Best Student Presentation Award Entry

Epitaxial strain in films grown on lattice-mismatched substrates plays a key role in tuning a wide range of physical and chemical properties of transition metal oxides (TMOs) through the modulation of oxygen vacancies. Strain has also shown potential for enhancing the thermoelectric (TE) properties of TMOs, enabling efficient heat-to-electricity conversion. Nevertheless, the effect of strain-mediated oxygen vacancies on TMO TE properties remains poorly understood. In this work, we explore the role of oxygen vacancies on the TE properties of epitaxial SrRuO3 (SRO) thin films by systematically varying strain using lattice-mismatched substrates to induce different strain states. In-situ X-ray diffraction reveals that compressive strain effectively reduces oxygen vacancy concentrations, thereby increasing charge carrier mobility without altering carrier density. compressively strained SRO films exhibit significantly improved electrical conductivity while maintaining consistent thermopower, resulting in a nearly threefold increase in power factor compared to relaxed films. Moreover, Time-domain thermoreflectance measurements demonstrate reduced thermal conductivity in compressively-strained films, leading to a greater than 50% improvement in the figure of merit when compared to bulk SRO. Our findings highlight the significant role of strain-controlled oxygen vacancies in modulating the TE properties of TMOs, providing a pathway to advanced materials design for high-temperature TE applications.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 97

Connecting electrochemical AFM techniques and traditional impedance spectroscopy

Volkmar Dierolf; Himanshu Jain; John Kaman (Lehigh University) Neus Domingo Marimon (Oak Ridge National Laboratory); Kyle Kelley (Center for Nanophase Materials Sciences, Oak Ridge National Laboratory)

Best Student Presentation Award Entry

A number of scanning probe-based techniques have been used to study electrochemical behavior of materials on the nanoscale, but it is difficult to apply a generalized description to their results. Crystalline Sb$_2$S$_3$, an optical and electrical phase change material, is an example of a material that shows a strong electrostatic response in scanning probe experiments, where glassy Sb$_2$S$_3$ shows no such response. Here, with a generalized approach, we show a close similarity between frequency-domain impedance spectroscopy measurements and time-domain electrical scanning probe experiments. It is shown that dynamics from surface probe techniques correspond to the same low-frequency dielectric behavior as measured in bulk, on the macroscale. Using the distinctly different electrical characteristics of glassy and crystalline Sb$_2$S$_3$, we show that it can be used to probe local dielectric characteristics with high sensitivity and spatial resolution. We identify characteristics of this material system that enables this comparison as well as the limitations of the approach.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 101

One-by-One Multimode Interferometer Filter on Thin-Film Lithium Niobate

Alison Haskin (University of Virginia); Devaaya Latta (University of Virginia)

Multi-mode interferometers (MMIs) are used as optical couplers in integrated photonic devices with applications in areas such as optical switching, astrophotonics and quantum information. We propose and demonstrate a one-by-one (1x1) MMI fabricated at the Oak Ridge Center for Nanophase Material Science (CNMS) using magnesium-doped thin-film lithium niobate on silicon oxide on silicon. This MMI can function as a compact, broadband filter to suppress transmission of selected frequencies. We demonstrate that this 1x1 MMI transmits 1550 nm light while successfully blocking 775 nm. The 775 nm transmission through a waveguide and the 1x1 MMI is 12-15 dB lower than through straight waveguides without the device. To demonstrate broadband applicability, tests were performed with a Continuously Tunable Laser (CTL), which showed that results were similar within 30 nm ranges centered around 775 nm and 1550 nm respectively. We present simulations of the electric field, as well as fabrication and measurement results.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 104

Andreev Mapping Studies of NbSe2 using Scanning Tunneling Microscopy

Benjamin Lawrie (Materials Science and Technology Division, Oak Ridge National Laboratory); Nirjhar Sarkar (MSTD, PSD)

Best Student Presentation Award Entry

We use non-contact Andreev reflection (NCAR) spectroscopy with scanning tunneling microscopy to map superconducting correlations in $NbSe_2$ with atomic resolution. Unlike point-contact Andreev reflection (PCAR), which lacks spatial control and can disturb the surface, NCAR operates in the tunneling regime, enabling systematic, non-invasive imaging of Andreev processes across individual atomic sites. By analyzing the decay of tunneling conductance with tip-sample separation, we detect spatial variations in Andreev reflection arising from orbital-dependent tunneling at Nb and Se atomic sites.

This variation is not explained by local density of states alone, and instead reflects how orbital symmetry and tip coupling modulate Andreev processes. Enhanced reflection near charge density wave (CDW) regions further reveals interplay between superconductivity and competing electronic order.

NCAR distinguishes superconducting gaps from other spectral features based on decay rate behavior, providing a complementary probe to conventional spectroscopic methods. It also allows access to higher-order Andreev processes as the junction approaches near-contact conditions.

This technique offers a sensitive, non-invasive method for probing microscopic aspects of superconductivity, with potential relevance for studying gap symmetry, orbital effects, and local electronic inhomogeneities in complex superconductors.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 106

Multiscale Study Of Artificial Quantum Lattices Formed On Cu(111) Surfaces Using CO Molecules

Christopher Coger (Auburn University); Panchapakesan Ganesh (Oak Ridge National Laboratory); Marcelo Kuroda (Auburn University)

Best Student Presentation Award Entry

Artificial lattices of carbon monoxide (CO) molecules on Cu(111) surfaces serve as powerful platforms for probing topological quantum effects relevant to quantum information science (QIS). In this multiscale computational study, we integrate density functional theory (DFT) and density functional tight-binding (DFTB) to characterize the electronic properties of honeycomb and Kagome CO lattices. Accurate DFT calculations of CO adsorption energetics and charge distributions validate and calibrate our DFTB parameterizations. Leveraging DFTB, we then simulate extended lattices, systematically varying molecular spacing and adsorption registries to assess their impact on surface density of states, band structure, and charge-transfer phenomena. Our results demonstrate that fine-tuning lattice parameters can markedly alter the electronic landscape and coherence properties of these artificial systems. These atomistic insights establish clear structure–property relationships and provide critical guidance for experimental efforts to develop robust, tunable CO-based platforms for next-generation QIS technologies.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 107

Integrating Freestanding Membranes for Band Gap Modulation in Gd-Doped CeO2

Habib Rostaghi Chalaki (University of South Carolina) Dongkyu Lee (University of South Carolina)

Best Student Presentation Award Entry

The development of advanced optoelectronic devices critically depends on the precise control of electronic and optical properties in functional materials. Among wide band gap oxides, ceria (3.0 ~ 3.2 eV) is a promising candidate due to its potential due to its tunable band gap, high chemical and thermal stability, and favorable ionic and electronic conductivity enabled by oxygen vacancies. However, conventional band gap engineering methods, such as chemical substitution, often introduce undesirable defects and degrade carrier mobility, ultimately limiting device performance. In this study, we demonstrate a novel strategy to engineer the band gap of Gd-doped CeO2 (GDC) using a freestanding membrane approach. Epitaxial GDC thin films with (001) and (111) orientations were fabricated via pulsed laser deposition on single-crystal $SrTiO_3$ substrates, utilizing a Ca-containing $Sr_3Al_2O_6$ (SCAO) water-soluble sacrificial layer and a polypropylene carbonate protective coating to ensure membrane integrity during release. Following complete detachment, the GDC membranes were transferred onto Al_2O_3 substrates. Interestingly, the (001) and (111) orientations resulted in flat and wrinkled surface morphologies, respectively, due to orientation-dependent lattice mismatch with SCAO. Despite these differences, electrical transport properties remained robust, suggesting the material's resilience to morphological variation. Importantly, surface wrinkling induced during fabrication led to a notable increase in the GDC membrane's band gap, offering a controllable optical effect relevant for device applications. This freestanding membrane approach enables precise band gap tuning while preserving conductivity and minimizing defect formation. Furthermore, the freestanding platform is compatible with a range of substrates and device architectures, facilitating scalable integration into advanced optoelectronic systems. Our results establish freestanding membrane-based band gap engineering as a promising alternative to traditional doping methods, setting a new paradigm for functional oxide material design.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 111

Adelites To Pyrochlores: A Hydrothermal Approach To Single Crystals Of Dimensional, Site-Ordered Quantum Magnets

Matthew Powell (Clemson University) Joseph Kolis (Clemson University)

Hydrothermal crystal growth uses an aqueous media for a slow dissolution of reactants followed by a piecewise-like nucleation of crystals. While slower than most conventional methods, this careful synthetic technique has long been known to give superior optical quality crystals of exceptional purity. Leveraging this crucial low-defect advantage, our group has long relied on a high-temperature and high-pressure hydrothermal technique to synthesize a series of dimensional quantum magnets. Unlike crystals grown via melt-based techniques, the hydrothermally prepared crystals are site-ordered and, more importantly, generally single domain. This allows relatively facile alignment of crystalline faces for anisotropic magnetization and neutron scattering experiments to probe the bulk and local magnetic phenomena. Dimensional quantum magnets rely on motifs such as linear 1D chains, trigonal 2D Kagome-like honeycombs and strips, and 3D tetrahedrons. As such, careful synthetic design and a site-ordered structure are paramount for accurate description of spin-exchange coupling interactions between magnetic centers, particularly in weakly-coupled rare-earth "liquid-like" spin systems where an unintended site defect (i.e., A-B site stuffing in pyrochlores) can induce an ordering event or inconsistent spin-exchange coupling constants. This talk will highlight the recent successes in preparing a new series of adelite-type AB(CO$_4$)(OH) structures and a refined synthesis of mm-sized A$_2$B$_2$O$_7$ rare-earth stannate pyrochlores. The adelites, with their linear-like 1D chiral chain motif and proposed cycloidal magnetic structure, offers a marked contrast with the highly ordered 3D tetrahedral arrangement of rare-earth ions in the stannate pyrochlores. Preliminary magnetization and neutron scattering studies will be discussed. Concluding remarks will highlight additional avenues for further study and synthetic design that will allow access to new structural analogs possessing their own unique magnetic structures.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 117

The Magnetic Property of BiFeO3 Thin Films Caused by Substrates

Warren Collins (Fisk University); India Gooch (Fisk University); Richard Mu (Tennessee State University); Lei Qian (Meharry Medical College); Hanna Terletska (Middle Tennessee State University); Akira Ueda (Fisk University, Tennessee State University); Ning Zhang (Fisk University)

bevel

Bismuth ferrite (BiFeO3) is a perovskite-based multiferroic material. We have fabricated layered multiferroic nanomaterials with a magnetron sputtering coater with a commercial BiFeO3 target as a source material and investigated the interface effects by using several kinds of substrates. The surface morphology was observed with a scanning electron microscope (SEM). Since there are several possible stoichiometries of bismuth ferrite compounds fabricated from the sputtering target of BiFeO3, we have analyzed the crystal structures of the bismuth ferrite compounds by the x-ray diffraction (XRD) and SEM with the energy dispersive X-ray spectroscopy (EDS). The magnetic polarization property caused by electric polarization was investigated by using several substrates such as indium tin oxide films, thin metallic films, and piezoelectric polymeric thin films (PVDF, polyvinylidene fluoride).

Acknowledgement: This work is supported by the U.S. Department of Energy, Office of Science, under award number DE-SC0025748 grant.

Topical Area: Hard matter: quantum, electronic, semiconducting materials

Poster # - 2 (Wednesday CNMS Poster Session)

All-Atom Modeling and Simulation of Bio-Polymer Interface: Dual Role of Antifouling Polymer Brushes

Seonghan Kim (CNMS) Zhefei Yang (CNMS); Ruben Millan Solsona (CNMS); Hanyu Wang (CNMS); Jacek Jakowski (CNMS); Panchapakesan Ganesh (CNMS); Scott Retterer (CNMS); Jan-Michael Carrillo (CNMS)

Antifouling polymers are highly valuable in a variety of applications, including antiviral coatings, targeted drug delivery, and marine coatings, where preventing unwanted protein adsorption is critical. Although extensive experimental studies have characterized polymer-protein interactions, computational studies remain limited due to the difficulty and complexity of integrating and investigating those two different components into a single system. This study presents molecular modeling and simulation of polyelectrolyte and polyzwitterionic brushes—poly(dimethylaminoethyl methacrylate) (PDMAEMA), poly(2-(N-oxide-N,N-dimethylamino)ethyl methacrylate) (PNOMA), and poly(2-(N-3-sulfopropyl-N,N-dimethylammonium)ethyl methacrylate) (PSBMA)—grafted onto α-quartz substrates. The brush models were developed to closely replicate experimentally synthesized brush samples and to provide detailed insights into structural and dynamical changes at the molecular level during protein adsorption. Using steered molecular dynamics simulations, we show that the PSBMA brush, due to its high local density, exhibits the greatest resistance to protein insertion. Ca root-mean-square deviation and interaction patterns analyses further reveal that PSBMA also induces the most significant destabilization of lysozyme, while PDMAEMA brush enhances protein stability through ion-mediated interactions. The PNOMA brush, while requiring the lowest force for protein adsorption, induces greater protein destabilization than the PDMAEMA brush primarily due to electrostatic repulsion caused by a shorter carbon spacer length. To the best of our knowledge, this study represents the first comprehensive and realistic model system—comprising nanomaterials, polymers, and proteins, specifically antifouling polyzwitterions and polyelectrolytes grafted onto a-quartz substrates via linkers. These findings highlight the dual role of antifouling polymer brushes: resisting protein adsorption and modulating protein structural dynamics, offering valuable insights for the rational design of next-generation antifouling materials.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 19 (Wednesday CNMS Poster Session)

UV-Activated Crosslinking of Polyzwitterionic Ultra-thin coatings for Enhanced Anti-fouling Performance

Rigoberto Advincula; Marea Blake; Marti Checa Nualart; Panagiotis Christakopoulos; Liam Collins; Spencer Cox (Oak Ridge National Laboratory); Benjamin Doughty; Jong Keum (Oak Ridge National Laboratory); Rajeev Kumar; Charini Maladeniya (Oak Ridge National Laboratory); Ruben Millan-Solsona (ORNL); Jennifer Morrell-Falvey; Scott Retterer (CNMS); Ilia ivanov (CNMS)

Antifouling strategies aim to prevent the adhesion and growth of unwanted biological organisms, such as bacteria, algae, and proteins, on material surfaces. Polyzwitterions, a subclass of polyampholytes bearing both positive and negative charges on each monomer, have shown exceptional antifouling capabilities due to their strong hydration layers and high surface energy, which together form a robust barrier against biofouling. In this study, we investigate ultrathin polyzwitterionic coatings based on poly(2-vinylpyridine propanesulfonate) (P2VPPS), synthesized via free-radical polymerization, for their antifouling performance. A benzophenone-functionalized silane was covalently attached to SiO_2 substrates to enable UV-induced crosslinking of spin-coated and drop-cast P2VPPS films. Controlled exposure to 365 nm UV light produced coatings with varied crosslinking densities and thicknesses. The resulting films were characterized using X-ray photoelectron spectroscopy, X-ray reflectometry, contact angle goniometry, atomic force microscopy, and sum frequency generation spectroscopy. Antifouling performance was evaluated through protein adsorption studies with β-casein using quartz crystal microbalance with dissipation (QCM-D) and neutron reflectometry, as well as microbial attachment assessments via multi-scale imaging of Pantoea sp. The results reveal that light-induced crosslinking significantly alters film structure and surface properties, with higher crosslinking levels correlating with increased thickness and protein retention. These findings highlight the tunability of polyzwitterionic coatings for antifouling applications through light-controlled crosslinking strategies.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 21 (Wednesday CNMS Poster Session)

Anti-Fouling and Charge-Tuning Surface Coatings Realized by N-oxide/Amine Polymer Brushes

Zhefei Yang (Oak Ridge National Lab) Hanyu Wang; Ilia Ivanov (CNMS)

N-oxides have been studied as a zwitterionic functional group with an extremely short dipole in the field of anti-fouling materials. In this work, we prepared polymer brushes containing N-oxides via SI-ATRP (surface initiated-atom transfer radical polymerization) and achieved brushes with controlled thickness for anti-fouling study. The achieved brushes were characterized on N-oxide content, salt and pH responsiveness, and biofouling resistance to proteins. In addition, we successfully demonstrated the reversible conversion between N-oxide brushes and tertiary amine brushes, enabling a controlled switch on surface properties, including surface charge, pH sensitivity and biofouling resistance. Overall, our work studied the N-oxide brush regarding synthesis strategy, brush stability, fouling resistance and controlled conversion with the tertiary amine brush, providing insights on surface coating with this novel anti-fouling zwitterion.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 22

Investigating Polyzwitterion and Polyanion Mixture Using Neutron Scattering: An Effective Polylelectrolyte Solution

Siao-Fong Li (ORNL) Jan Michael Carrillo (ORN L); Panagiotis Christakopoulos; Changwoo Do (Oak Ridge National Laboratory); Jong Keum (Oak Ridge National Laboratory); Rajeev Kumar; Piotr Zolnierczuk

Best Student Presentation Award Entry

Polyzwitterions (PZ) and polyanions (PA) mixtures attract a surge of interest due to their broad applications. Here, employing molecular dynamical simulations and neutron scattering experiments, we investigate the structures and dynamics of poly(3-(2-vinyl-1-pyridiniumyl)-1-propane sulfonate) (P2VPPS) and sodium poly(styrene sulfonate) (NaPSS) solutions in dilute regimes. Both simulation and experiment results reveal the emergence of a peak in the PZ structure factor under various polymer concentrations and molecular weights. We interpret this feature as the outcome of PZ-PA complexations, leading to an interesting concept—effective polyelectrolyte solutions. The idea suggests that PAs dominate such systems. While this idea qualitatively accounts for the observed de Gennes narrowing in the PZ dynamical structure factor, the dynamics remain qualitatively distinct from those of pure PA solutions, necessitating the theoretical development of dynamics. This work provides insights into PZ-PA systems and motivates more comprehensive future studies.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 23

Linear Reciprocating Tribometer for In Situ Neutron Reflectometry of Soft Matter

Angela Pitenis; Kathryn Shaffer (University of California, Santa Barbara) Ahmed Tariq Al Kindi; Rebecca Anderson; Brendan Louie Bagorio; Julia Ong; Roger Pynn; Andrew Rhode; Juan Manuel Urueña; Erik Watkins

Best Student Presentation Award Entry

Neutron reflectivity excels at elucidating structure of soft mater interfaces. Sample environments have previously been used to study soft matter interfaces at rest, in compression, and subject to non-uniform shear stress. This work showcases a new custom tribometer design for conducting in situ measurements of forces during dynamic compression and linear sliding motion coupled with neutron reflectometry to observe structural changes within soft matter. Design considerations for safety, neutron transmission, and sample positioning are discussed. Preliminary neutron reflectivity data from compression and sliding tests of polyacrylamide hydrogels are also presented.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 25

Morphological Studies of the Ordering of Block Copolymer Thin Films in Applied Electric Field using Neutron Reflectometry

Candice Halbert (Department of Chemistry, University of Tennessee; Spallation Neutron Source, Oak Ridge National Laboratory) S. Michael Kilbey (Department of Chemistry, University of Tennessee,); Bradley Lokitz (CNMS/ORNL); Andre Parizzi (Spallation Neutron Source, Oak Ridge National Laboratory,)

Block copolymers (BCPs) are polymeric analogs of surfactants that form three-dimensional, ordered structures in the bulk and in thin films. Ordering of BCPs thin films is important as nanostructured materials find application in diverse areas such as chip-based (bio)sensors, battery electrolytes, and optoelectronic devices. It is well-known that the organization and alignment of a microphase separated block copolymer thin film can be enhanced by the application of an electric field, resulting in alignment parallel to the direction of the electric field (here, perpendicular to the surface). The ordering depends on several factors, including field strength, the dielectric constant of each polymer block, time, and interfacial energy between the contacting block and the solid support. In this study deuterated polystyrene-block-poly(ethylene oxide) (dPS-b-PEO) was spin-coated from a non-selective good solvent, creating disordered films that were tens of nanometers in thickness. These films were then subjected to an electric field and elevated temperatures, resulting in microphase-separated lamellae structures. Neutron reflectometry was used to determine the morphological structures of the BCP thin films by probing the laterally-averaged depth-profile of the dPS-b-PEO films. It was found that the formation of lamellae domains aligned both parallel and perpendicular to the solid support surface in dPS-b-PEO thin films is dependent on the electric field strength, temperature, and time. We plan to present the neutron reflectivity of block copolymer thin films as a function of applied electric field strength and temperature.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 44

Resolving Nanoplastic Aggregation and Size at Soil-Water Interfaces via Small Angle Neutron Scattering (SANS) and Ultra-SANS (USANS)

Douglas Hayes (University of Tennessee Knoxville) Abimbola Ajibola (University of Tennessee Knoxville); Anton Astner (Oak Ridge National Laboratory); Barbara Evans (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Sai Venkatesh Pingali; Volker Urban (Neutron Scattering Division, ORNL)

Best Student Presentation Award Entry

The presence of nanoplastics (NPs) in the environment represents a major challenge due to potential soil/water contamination, and the transport of toxic substances. Their relatively small size (1–1000 nm) and high surface reactivity results in a wide range of complex interactions with heavy metals, organic matter, and biological substances. Understanding these interactions involves investigation at complex interfaces, such as those between soil and water. While conventional characterization methods such as microscopy can adequately study plastic particles at the microscale, they often lack the adequate resolution to study them at the nanoscale where challenges such as extremely low NP concentrations and signal interference from the environmental matrix (e.g., soil and organic matter) are prominent. In this study we investigated structure and aggregation behavior of suspensions of NPs derived from mechanically treated plastic films and microparticles of artificial soil, vermiculite (V), in water, as would form near soil-water interfaces, through Small Angle Neutron Scattering (SANS) and Ultra-SANS (USANS) at Oak Ridge National Laboratory. We employed suspensions of NPs composed of different polymeric materials and containing adsorbed biofilm components (e.g., humic acid and proteins) and V in water at different concentrations and ex-situ stirring times. By utilizing neutron contrast matching techniques, we matched out the signal attributable to V or adsorbed biofilm components, giving insight into the particle size distribution, agglomeration, and mobility of NPs under environmentally applicable conditions. The results from this study showed that the NPs formed had two distinct subpopulations: a smaller and a larger NP fraction with mean diameters of ~ 200 and 850 nm respectively. It was also observed that the presence of V in the suspension, while emulating environmental conditions facilitated aggregation and further size reduction of NPs through abrasive forces between particles. Our findings explain the role of soil components in determining NP fate and transport.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 53 (Wednesday CNMS Poster Session)

Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent Molecular Dynamics

Jan Michael Carrillo (ORNL)

Performing simulations of soft matter systems, particularly molecular dynamics simulations, often involves coarse-graining the system's description while preserving the particle nature of the model. This approach includes implicitly modeling the solvent as random forces acting on the particles, such as using a Langevin thermostat in an NVT ensemble simulation. This method reduces computation costs and speeds up the evolution of large-scale structures or features of the model due to the shallower energy barriers in the free energy landscape. However, in certain scenarios, explicitly modeling the solvent becomes necessary. For example, the inclusion of a polar solvent in the model allows for a more accurate representation of these systems at higher concentrations, where the assumptions of a continuum dielectric medium and screened hydrodynamics break down. It is also necessary to use explicit solvent in nonequilibrium molecular dynamics simulations for studies under mechanical deformation or an electric field. We present soft matter systems where the solvent was explicitly included in the model, including a polyelectrolyte in semi-dilute solutions under shear, and a lipid bilayer with a zwitterionic lipid head in a dipolar solvent with added salts and an applied oscillating electric field, causing a charge imbalance and enabling the membrane to act as a capacitor.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 56 (Wednesday CNMS Poster Session)

Can Martini Coarse-Grained Models Capture Antifouling Behavior Of Polyzwitterionic Brush Coatings?

Christopher Walker (Oak Ridge National Laboratory) Jan Michael Carrillo (ORN L); Seonghan Kim (CNMS)

Biofouling has widespread implications for everyday materials, including biomedical devices, personal protective equipment, and marine coatings, leading to performance degradation and high costs. Polyzwitterionic brush coatings are known to exhibit antifouling behavior due largely to a strongly coupled hydration layer, yet the detailed mechanism is not fully understood. Moreover, only a handful of polymer chemistries have thus far been identified as highly antifouling.

Molecular dynamics (MD) simulations are a vital tool for studying polymer-protein interactions at angstrom-scale resolution, enabling both screening of polymer chemistries for antifouling properties, and interpreting experimental results indicating antifouling behavior. Coarse-grained (CG) simulations, in which atoms are grouped into effective interaction sites, lead to substantial gains in computational efficiency and allow for accessing microsecond timescales in large polymer systems.

In this work we present new Martini CG models for a series of polyelectrolyte and polyzwitterion chemistries compatible with Martini 2 polarizable water. CG brush models are validated by comparing density profiles and pair correlation functions against all-atom systems. Finally, adsorption free energies of lysozyme into the brushes are computed via metadynamics. We assess whether the models can capture the expected effects of brush chemistry and salt on antifouling behavior.

Acknowledgements:

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Topical Area: Soft matter: polymers, and complex fluids

Poster # - 64 (Wednesday CNMS Poster Session)

Sustainable Soft Matter Systems: Bioderived nanomaterials and Biocatalysis

Yue Yuan (Oak Ridge National Laboratory) Victor Sharma

The urgent need for sustainable chemical synthesis and material innovation has accelerated research at the intersection of soft matter science, bio-derived nanostructures, and green chemistry. This presentation demonstrates ongoing research at Macromolecular Nanomaterials Group on sustainable soft matter systems that leverage biological feedstocks and enzymatic processes to advance circular polymer technologies.

We first demonstrate the use of mycelium-derived polyscacchirdes as a renewable and structurally robust filler for polymer composites, enabling enhanced mechanical performance while maintaining biodegradability. With low loading (< 5% wt.), the reinforcement effect of these particles in polyvinyl alcohol (PVA) hydrogel is comparable to that of nanoscale cellulosic particles (CNCs) and graphene oxides (GOs) additives—of which typically require harsh conditions such as strong acids and elevated temperatures during synthesis. Variations in chemical composition and particle morphology (fibrous structures vs. dense particles) among mycelium from different fungal species contribute to significantly different reinforcement outcomes. In some cases, the biosynthesis and chemical extract approaches used for filler preparation also enable polyscacchirdes deuteration for contrast match technique in neutron scattering experiments. In addition to hydrogel, we present strategies for electrospinning bioderived molecules—such as lignin derivatives, cellulose nanocrystals, and biosynthesized polymers—into functional nanoscale fibers with tailored morphology and functionality. Finally, we highlight research on the biocatalytic synthesis of aliphatic polyesters in vitro via lactone ring opening polymerization using hydrolases as catalysts in a biphasic system. This approach offers mild, selective, and solvent-efficient routes to polymer formation. The microstructures of resulting block copolymers can be tuned through enzyme selectivity, yielding materials with distinct physical properties such as crystallinity.

Together, these approaches from synthesis to material processing illustrate a cohesive vision for integrating materials science with biology to design next-generation soft matter systems that are both high-performance and sustainable.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 75

Small-Angle X-ray Scattering (SAXS) and X-ray Reflectometry (XRR) at CNMS and NSD: Enabling Structural Characterization and X-ray–Neutron Synergy

Jong Keum (Oak Ridge National Laboratory)

Small-Angle X-ray Scattering (SAXS) and X-ray Reflectometry (XRR) are powerful characterization techniques available at the Center for Nanophase Materials Sciences (CNMS) and the Neutron Scattering Division (NSD) at Oak Ridge National Laboratory (ORNL), enabling detailed nanoscale structural analysis of a wide range of materials. SAXS provides quantitative insights into the size, shape, and hierarchical organization of nanostructures in solution, bulk, and thin-film forms. XRR, in turn, probes electron (X-ray scattering length) density profiles and interfacial roughness in layered systems with sub-nanometer resolution. These complementary techniques are central to CNMS and NSD science in areas such as soft matter, hybrid interfaces, and quantum materials, and are broadly applicable to polymers, nanocomposites, biomaterials, and thin films. This presentation will highlight the SAXS and XRR capabilities and sample environments available across CNMS and NSD, with illustrative examples from user projects that demonstrate their scientific impact. Particular emphasis will be placed on the complementary nature of X-ray and neutron scattering techniques, and on the role of SAXS and XRR as high-throughput tools for early-stage structural screening prior to neutron experiments—specifically, small-angle neutron scattering (SANS) and neutron reflectometry (NR). These integrated approaches significantly enhance the efficiency, focus, and scientific return of subsequent measurements at the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR), supporting streamlined and synergistic X-ray–neutron workflows for both CNMS and NSD users.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 76

Measuring And Modeling Non-Gaussian Deformations Of Topologically-Complex Polymers Using In Situ Capillary Rheo-SANS

Anukta Datta; Matthew Helgeson (UC Santa Barbara); Siobhan Powers (University of California, Santa Barbara); Patrick Underhill (RPI); Xiaoyan Wang (RPI)

Best Student Presentation Award Entry

Macromolecular topology provides an opportunity to engineer polymers that provide orthogonal control over rheological performance and mechanical stability in high-shear rate applications. In this work, we combine topology-controlled polymer chemistry with in situ neutron scattering measurements in a high-shear capillary device (capillary rheo-SANS) that can probe the rheology and microstructure of polymers in shear flows exceeding rates of 106 s-1. We synthesize and study high molecular weight, low-dispersity, topology-defined poly(methyl methacrylate-co-stearyl methacrylate) polymers with linear and star-shaped architectures for model studies of flow-induced deformation in dilute solutions at extreme shear rates. The resulting scattering is interpreted using a new modeling framework, the Gram-Charlier analysis of polymer scattering (G-CAPS) that fingerprints polymer conformations through non-Gaussian moments of the segment density distribution. Brownian dynamics simulations are used to show that the moments extracted from G-CAPS can be used to distinguish effects of finite extensibility in large strain-rate flows. We show that these measures, when extracted from capillary rheo-SANS measurements, provide a molecular-level explanation for differences in rheology and mechanical stability between linear and star polymers, as well as molecular-weight dependent effects of finite extensibility. More generally, we anticipate that capillary rheo-SANS in combination with G-CAPS will provide powerful new tools to engineer polymers rheology through macromolecular architecture.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 82

Integrated in-situ Techniques for Studying Protein Adsorption Behavior on Polymer Thin Films

Marea Blake; Liam Collins; Benjamin Doughty; Maya Endoh (Stony Brook University); Aiden Gauer; Tad Koga (Stony Brook University); Scott Retterer (CNMS); Hanyu Wang; Marko Zimic (Stony Brook University)

Best Student Presentation Award Entry

The ongoing challenge of preventing disease transmission underscores the need for materials that reduce pathogen adhesion and proliferation. Medical devices such as catheters and implants are prone to biofilm formation, which is often initiated by protein adsorption. While much is known about protein adsorption on rigid surfaces, significant gaps remain regarding polymer surfaces, where flexibility and mobility add complexity. Traditional models fail to explain our lab's findings, particularly for protein adsorption on neutral polymers. Previous ex-situ data from our group shows that adsorption is positively correlated on film thickness independent of polymer chemistry [1]. Additionally, polymer thin films show strong antifouling behavior for thicknesses under 20 nm. Here, we present new insights into protein adsorption mechanisms on polystyrene (PS) thin films. Films were made at different thicknesses from the flattened layer (2-3 nm) up to 100 nm. We present new in-situ experiments to further elucidate the interactions that drive protein adsorption on polymer surfaces using bovine serum albumin (BSA) and human plasma fibrinogen as model protein. We combine neutron reflectivity (NR), quartz crystal microbalance (QCM), sum frequency generation (SFG), and atomic force microscopy (AFM) techniques to study adsorption kinetics, protein/polymer binding, protein orientation, and protein penetration at the polymer interface.

1. Salatto D. et al. Macromolecules 2020 53 (15), 6547-6554.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 88 (Wednesday CNMS Poster Session)

The Development of novel polymers: using in situ/operando neutron reflectometry to unveil structure-function relationships

Hanyu Wang; Jim Browning (ORNL); Riccardo Candeago (University of Illinois, Urbana Champaign); Rajeev Kumar; Scott Retterer (CNMS); Xiao Su (Chemical and Biomolecular Engineering); Zhefei Yang (Oak Ridge National Lab)

Neutron has many extraordinary properties, e.g., highly penetrating, particularly sensitive to light elements like hydrogen and carbon, power of polarization and magnetic moment. All these characteristics make neutrons excellent probes of materials, providing details about the structure and motion of atoms that cannot be easily obtained with other research techniques. Neutron reflectometry (NR), a neutron scattering technique, is a powerful tool to investigate surface and interfacial structures of thin films in a non-destructive and non-invasive fashion. The Liquids Reflectometer (LR) at the Spallation Neutron Source at Oak Ridge National Laboratory measures specular neutron reflectivity in a horizontal sample geometry, and tracks changes of layer thickness, scattering length density, and roughness as a function of depth. LR provides valuable information over a wide variety of scientific and technological applications, such as, interfacial reactions in energy conversion and storage materials, phase separation in polymer films, surfactants at interfaces, protein adsorption, biological membranes in intermolecular interaction, and so on. The exceptional sample environment at LR offers the capability to conduct in situ electrochemistry to probe the morphological and structural changes at the solid/liquid interfaces during operation as a function of chemical and electrochemical gradients over time. Furthermore, event mode data collection at LR can be carried out continuously over a reduced Q range and binned into 60-second (or even shorter) intervals. The improved time resolution of the NR measurement can help elucidate the kinetic behavior of surface/interfaces under dynamic conditions and bring a unique perspective to equilibrium studies. Two specific examples of applications in novel polymer development by using in situ/operando NR will be presented. The example studies shed light on fundamental understanding of the structure-function relationships of the polymers. NR plays a key role in creating new, and more efficient polymer systems through rational design of the structure and operating conditions.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 105

Mechanochemical Synthesis of Naloxone-Poly (Lactic Acid) for Drug Delivery

Sandun Bogahawaththa; Kasthuri Dias (Graduate Research Assistant, Bredesen Center, University of Tennessee-Oak Ridge Innovation Institute) Mohammad A. Ebqa'ai (Assistant Professor, Department of Chemistry, Physics, & Engineering, Cameron University); Toby L. Nelson (Research Associate Professor, University of Tennessee-Oak Ridge Innovation Institute)

Best Student Presentation Award Entry

Poly(lactic acid) (PLA) is a biodegradable polymer that is used widely in biomedical applications due to its sustainability and biocompatibility. Naloxone is an opioid antagonist that is efficacious in the emergency treatment of opioid overdoses. However, its effectiveness in overdose reversal is limited by its rapid metabolism and short half-life, which require repeated dosage. We have created a mechanochemical technique that uses a one-step anionic ring-opening polymerization of lactide to create naloxone-linked poly(lactic acid) (NLX-PLA) nanoparticles in order to overcome this limitation. Compared to conventional bulk polymerization, this method afforded more stable nanoparticles and a higher naloxone drug loading. Our research indicates that mechanochemistry can be used to build scalable and green drug delivery systems, which is a feasible approach for treating opioid overdoses.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 108

Multi-scale Structural Effects of Co-solvent Pretreatment of Lignocellulosic Biomass for Enhanced Biorefinery Efficiency

Anton Astner Sai Venkatesh Pingali; Barbara Evans (Oak Ridge National Laboratory); Hugh O'Neill (Oak Ridge National Laboratory); Manjula Senanayake (Clemson university); Austin Conte; Brian Davison

Efficient lignocellulosic biomass utilization is essential for sustainable biofuel and bioproduct manufacturing within a biorefinery framework. However, the inherent recalcitrance of plant cell walls - caused by densely packed cellulose fibrils embedded in a lignin-hemicellulose matrix - presents a significant obstacle to effective industrial-scale pretreatment. Therefore, cosolvent-pretreated biomass was characterized using small-angle neutron scattering (SANS) technique to determine structural parameters to predict the most efficient cosolvent pretreatment by combining with machine learning approaches. SANS was employed to probe the nanoscale structural evolution of solvent pretreated poplar biomass subjected to a comprehensive matrix of 163 experimental runs spanning three solvent severity levels (strong, medium, weak) and three varying pretreatment severities levels (2.07, 2.73, 2.95) based on temperature, residence time, and sulfuric acid concentration. Key structural parameters, including the radius of gyration (Rg), power-law exponent (P), and Guinier and Porod scalars (G, B) were extracted to quantitatively describe changes in size distribution of cellulose microfibril diameter, lignin/hemicellulose aggregate particle size, surface roughness of micron-sized structures like cell lumen. Statistical analysis revealed that solvent severity had a significant influence ($p = 0.05$) on smaller structural features, such as cellulose microfibril radius Rg, indicating that solvents strongly modulate biomass nanostructure, while pretreatment severity driven by sulfuric acid concentration and temperature did not result in statistically significant Rg difference, as well as increase in surface roughness. By establishing robust correlations between pretreatment conditions and nanoscale structural signatures, the study provides a predictive foundation for optimizing carbohydrate accessibility and yield using the cutting-edge SANS technology combined with advancing biorefinery technologies.

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 110

CMOS-Compatible Carbonization of 3D-Printed Nanoelectrodes via Global Annealing and Localized Joule Heating for Cell-on-CMOS Biosensing

Farin Rahman (University of Tennessee, Knoxville) Nickolay Lavrik (Center for Nanophase Materials, Oak Ridge National Laboratory); Nicole McFarlane (University of Tennessee, Knoxville)

Best Student Presentation Award Entry

This work details the development of a cell-on-CMOS biosensor system that integrates fully carbonized 3D-printed nanoelectrodes with CMOS readout circuits for real-time cellular monitoring. The electrodes were fabricated using a platinum-on-titanium metal stack, chosen for its superior adhesion and thermal stability. Electrode layouts were designed in the industry-standard GDSII format and patterned onto 100 mm silica wafers through contact photolithography and metal lift-off techniques. These wafers were diced into 25 mm × 25 mm chips for further processing.

To enable three-dimensional nanoscale sensing, bridge-on-pillars (BoP) microstructures were fabricated using two-photon polymerization (2PP) with the Nanoscribe Photonic Professional GT tool and IP-S photopolymer. After printing, uncrosslinked polymer residues were removed by immersion in SU-8 developer, followed by isopropanol washing and nitrogen drying. The printed structures underwent a two-step thermal annealing process, similar to standard carbon fiber manufacturing. Initially, the polymer was stabilized by heating in ambient air at 340°C for 10 minutes to initiate oxidation. Complete carbonization usually requires temperatures exceeding 900°C, which are incompatible with CMOS chips due to their limited thermal tolerance (~400–450°C). To address this, carbonization was carried out in argon at 500–600°C for 8–15 hours using a rapid thermal processing tool, maintaining CMOS compatibility.

In current work, electrical characterization of the thermally annealed, partially carbonized BoP structures was performed over a month using a FormFactor point probe system. Measurements conducted at a fixed 100 V bias over a temperature range of 20°C to 270°C showed that the structures had noticeable structural shrinkage (Fig.[1]) alongside consistent exhibition of nanoampere-level conductivity (Fig.[1]). Some mechanical failures were observed, likely due to the intrinsic fragility of these suspended nanoscale architectures. Future research will investigate the mechanisms behind these failures, hypothesizing that mechanical stress during handling or thermal cycling contributes to the degradation.

[1]: https://drive.google.com/drive/folders/1tA2c7HUpeKkEIzko7Ln-Hxc62YJPr_35?dmr=1&ec=wgc-drive-hero-goto

Topical Area: Soft matter: polymers, and complex fluids

Poster # - 113

Electrospun Multiferroic Nanocomposites: PVDF-TrFE Fibers Doped with Iron Oxide Nanoparticles.

Joshua Adjei - Yeboah (TIGER Institute, Tennessee State University, Nashville TN 37209) Axel Hoffmann (Illinois Materials Research Science and Engineering Center, University of Illinois at Urbana-Champaign, Urbana, IL 61801); Richard Mu (TIGER Institute, Tennessee State University, Nashville TN 37209); Fatima Tuz Zahra (TIGER Institute, Tennessee State University, Nashville TN 37209); Akira Ueda (Department of Life and Physical Sciences, Fisk University, Nashville TN 37208); Lei Zhu (TIGER Institute, Tennessee State University, Nashville TN 37209)

Best Student Presentation Award Entry

Multifunctional polymer nanocomposites are increasingly being explored for next-generation flexible electronics and smart sensing and energy harvesting applications. In this study, we report the fabrication and morphological optimization of electrospun nanofibers based on the ferroelectric copolymer poly(vinylidene fluoride–trifluoroethylene) (PVDF-TrFE), doped with magnetic iron oxide (Fe_3O_4) nanoparticles. The goal is to develop multifunctional systems exhibiting both piezoelectric and magnetic properties, paving the way toward magnetoelectric coupling in flexible platforms. A series of experiments were conducted using PVDF-TrFE solutions (80:20 molar ratio) in an acetone:DMF solvent system, with Fe_3O_4 introduced in both powdered and colloidal forms. Challenges such as nanoparticle agglomeration and solvent incompatibility (especially with toluene-based colloids) were addressed through probe sonication and viscosity tuning via polymer concentration adjustments (10–18 wt%). The influence of electrospinning parameters—voltage (10–25 kV), flow rate, needle-to-collector distance, and needle gauge—on fiber morphology was systematically evaluated using scanning and transmission electron microscopy (SEM/TEM). Energy dispersive X-ray spectroscopy (EDS) confirmed the presence of Fe_3O_4, although dispersion remained non-uniform. Our findings show that nanoparticle doping significantly affects fiber morphology and enhances the piezoelectric response by increasing the electrical conductivity of the spinning solution. Optimized conditions yielded uniform, bead-free fibers with reduced diameters. Despite partial success in achieving nanoparticle dispersion, evidence of magnetoelectric coupling remains to be established. This work contributes to the growing body of multiferroic material research aimed at integrating electrical and magnetic functionalities in polymer nanofibers for emerging applications in wearable devices, energy harvesting, soft robotics, and adaptive sensing.

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Topical Area: Soft matter: polymers, and complex fluids

Poster # - 119

Recent Instrument Upgrades of the Triple-Axis Spectrometer VERITAS

Wei Tian (Oak Ridge National Laboratory | SNS | HFIR)

VERITAS (HB-1A) located in the thermal beam room at HFIR, recently completed a major upgrade to rebuild the entire instrument. The instrument utilizes a double-bounce pyrolytic graphite monochromator system and a pyrolytic graphite analyzer to produce an intense, clean beam at l = 2.38 Å with low background and an excellent signal-to-noise ratio. The upgrade resulted in a >4x signal gain and enables two new capabilities on VERITAS: a new four-circle goniometer capability which has been successfully commissioned and is now available in the user program; and a small 2D detector option at the analyzer position which is under development and will become available soon. With its large Q-coverage (0.1 to 4.8 Å-1) and open sample position, VERITAS is optimized for magnetic diffraction studies supporting a wide range of complex sample environments.

Topical Area: