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Tuesday Plenary Session

Ferroelectrics Everywhere: New Material Discovery by Engineered Instabilities

Jon-Paul Maria (Pennsylvania State University)

Ferroelectricity in wurtzite-based crystals was observed in 2019 and immediately introduced exciting opportunities to explore and discover new structure-property relationships in novel formulation spaces, and to investigate new integration and device implementations given new process compatibilities. The seminal discovery of ferroelectric Al1-xScxN initiated this excitement and was followed by comparable observations of polarization reversal in the structurally similar Al1-xBxN and the Zn1-xMgxO systems. These observations lead one to speculate that ferroelectricity might be found much more broadly, even “everywhere”, by introducing the appropriate disorder in a variety of hosts. The presentation will begin with a brief history of ferroelectricity with specific attention to the last 10 years where this important property was discovered in new oxide and nitride crystals, and how these lead the community’s thinking about finding more. The remaining content will focus on the structure-process-property relationships in the B-substituted AlN and Mgsubstituted ZnO wurtzite systems. The B-substituted materials exhibit square hysteresis loops with polarization values between 150 µC/cm2 and 120 µC/cm2 when boron concentrations range between 2% and 15% respectively. Coercive field values fall with additional boron, from 5.5MV/cm to about 5 MV/cm at B saturation. Bandgap values are approximately 5 eV or above in all cases. Material can be prepared between 100 °C and 350 °C with very little difference in electrical properties. Case studies will be shown using metallic, metal nitride, and doped Si bottom electrodes. In the best cases, capacitors can be prepared down to 10 nm thickness while still exhibiting ferroelectric switching. Below 25 nm, however, leakage current becomes problematic during low frequency hysteresis measurements. First principles calculations that rationalize the unit cell volume, bond angle distribution, and remanent polarization will be presented. Comparable results will be presented for the Zn1-xMgxO system. Between ~7% and 45% Mg substitution, square hysteresis loops with remanent polarization values near 100 µC/cm2 are readily achieved. In comparison to AlBN, coercive field values for ZMO can be less than 2.0 MV/cm. The presentation will also include examples where proximity effects in layered ZnO/Zn1-xMgxO, AlN/Al1-xBxN, and Zn1-xMgxO/AlN heterostructures can induce switching in pure ZnO and AlN layers. The presentation will finish with a summary of accomplishments and challenges that the community is observing for these novel ferroelectric compositions and an outlook regarding opportunities to shepherd their integration into device applications."

Hard Matter: Quantum, electronic, semiconducting materials (Tuesday 1:30-4:00 PM)

Spin splitting in the chiral magnet EuAuSb

Jennifer Sears (Brookhaven National Laboratory)

EuAuSb is a layered Dirac semimetal which exhibits a variety of unusual transport phenomena, including chiral magnetic and topological Hall effects. The topological Hall effect in particular is seen only in the magnetically ordered phase, suggesting that symmetry breaking due to magnetic order may be important for understanding electronic behavior. We have therefore collected single-crystal neutron diffraction measurements and identified an incommensurate helical order in which ferromagnetic Eu2+ layers rotate in-plane by ~120° from one layer to the next [1]. An in-plane magnetic field distorts the incommensurate order, eventually leading to a first order transition to a commensurate state, followed by the field polarized state. In the field range where topological Hall effect is at a maximum, we observe a suppression of the in-plane ordered moment and consider possible explanations for this observation. The observed magnetic order also breaks both parity and time-reversal symmetries, leading to a loss of spin degeneracy in the band structure even in the absence of spin-orbit coupling. We compare this spin-splitting to that seen in the collinear alter magnets, as well as the more recently studied coplanar magnetic materials termed p-wave or odd-wave magnets.

[1] J. Sears, Juntao Yao, Zhixiang Hu, Wei Tian, Niraj Aryal, Weiguo Yin, A. M. Tsvelik, I. A. Zaliznyak, Qiang Li, and J. M. Tranquada, EuAuSb: A helical variation on altermagnetism, arXiv:2505.00081
(2025)

Work at Brookhaven is supported by the OWice of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704"

Pentagonal all-in-all-out antiferromagnetic chains in NaMn6Bi5

Madalynn Marshall (Kennesaw State University); Raimundas Sereika (Department of Physics, University of Alabama, Birmingham at Alabama); Wenli Bi (Department of Physics, University of Alabama, Birmingham at Alabama); Randy Fishman (Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA); David Parker (Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA); Huibo Cao (Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA)

Quasi-one-dimensional systems have garnered significant attention owing to the exotic properties they can host including superconductivity, charge density waves, topological spin excitations and more. Pressure-induced superconductivity has been realized in a new family of Mn-based Q1D materials, AMn6Bi5 (A = K, Rb, Cs, Na), with unique [Mn6Bi5]−1 double-walled columns. The smallest countercation Na+ yields the highest chemical pressure experienced in this family, reducing the Mn interatomic bond lengths and enhancing the metallicity and magnetic frustration within the Mn pentagonal antiprisms, thus, driving NaMn6Bi5 closer to the high-pressure superconducting phase. Distinct from the single magnetic transition in other family members, NaMn6Bi5 goes through multiple magnetic transitions at TN1 ~88 K, TN2 ~52 K and TN3 ~48 K. In this talk I will present the findings of the unique low temperature, below TN3 ~48 K, noncolinear “all-in-all-out” pentagonal antiferromagnetic order and high temperature in-plane moment dispersed pentagon phase in NaMn6Bi5 determined from single crystal neutron diffraction. The low temperature “all-in-all-out” state exhibits spins pointing all towards or away from the center of the pentagon and alternating down the Mn pentagonal antiprism columns along the b axis. The innermost central Mn-site continuously shows no/negligible ordered moment, resulting from the magnetic frustration within the Mn pentagonal antiprisms and nearly metallic bond distances. High pressure X-ray diffraction up to 18.5 GPa revealed no additional lattice transition, indicating the magnetic variation under pressure is highly relevant to the high-pressure superconducting phase found in this family. This investigation has, therefore, shed new light on the rare one-dimensional Mn-based superconductors.

Observation of Heeger's Susceptibility Divergence near the CDW Transition in ErTe3 with Momentum-Resolved EELS

Peter Abbamonte (University of Illinois Urbana-Champaign)

A charge density wave (CDW) is a phase of matter characterized by a periodic modulation of valence electron density coupled to a lattice distortion. In 1979, Alan Heeger predicted that the CDW transition should be accompanied by a divergence in the dynamic charge susceptibility, but this effect has never been observed experimentally. In this talk I will present momentum-resolved inelastic electron scattering (EELS) measurements of the charge susceptibility in the canonical CDW material ErTe3 with meV energy resolution. The valence band electronic excitations exhibit relaxational dynamics that are described well by a diffusion model, with the diffusivity peaking just below the critical temperature. Additionally, I will show, for the first time, a divergence in the real part of in the static limit ( )—a long-predicted hallmark of CDWs. Unexpectedly, this divergence occurs as with only a weak thermodynamic signature at the transition temperature. Our study necessitates a reexamination of the traditional description of CDW formation in quantum materials.

*D. Chaudhuri, et al., arXiv:2411.14746 (to appear in PNAS)

Engineering of magnetic chalcogenide interfaces guided by polarized neutron reflectometry

Hang Chi (University of Ottawa)

Significant recent effort has been devoted in understanding the geometric aspects of condensed matter [1]. The marriage of topology and magnetism at disparate quantum interfaces, guided by polarized neutron reflectometry (PNR), constitutes an exciting arena for developing novel memory, logic and information technologies. We introduce quasi-two-dimensional (2D) magnetic transition metal chalcogenide Cr2Te3 grown by molecular beam epitaxially (MBE) as an emerging platform for spin-orbit driven Berry phenomena [2]. A unique temperature/strain modulated sign reversal of the anomalous Hall effect has been discovered and attributed to nontrivial Berry curvature physics [3]. The versatile interface tunability of Cr2Te3, when hybridized with a topological insulator [4], offers new designs for topological devices [5]. Furthermore, we observe nonreciprocity in supercurrent transport and demonstrate strong field-free superconducting diode effect in magnetic insulator/superconductor bilayers [6]. These heterostructures enable new computing regime with low energy cost, mitigating Joule heating with dissipationless supercurrent, well suited for high demanding data centers. The PNR technique is ideal in advancing the understanding of magnetic surfaces and interfaces, for exciting development of topological and superconducting spintronics.

References:

[1] H. Chi et al., Progress and prospects in the quantum anomalous Hall effect, APL Mater. 10, 090903 (2022).
[2] S. Kwon et al., Evolution of Berry phase and half-metallicity in Cr2Te3 in response to strain, filling, thickness, and surface termination, Phys. Rev. B 109, 134430 (2024).
[3] H. Chi et al., Strain-tunable Berry curvature in quasi-two-dimensional chromium telluride, Nat. Commun. 14, 3222 (2023).
[4] P. J. Taylor et al., Magnetotransport properties of ternary tetradymite films with high mobility, Mater. Today Phys. 46, 101486 (2024).
[5] Y. Ou et al., Enhanced Ferromagnetism in Monolayer Cr2Te3 via Topological Insulator Coupling, Rep. Prog. Phys. in press (2025).
[6] Y. Hou et al., Ubiquitous Superconducting Diode Effect in Superconductor Thin Films, Phys. Rev. Lett. 131, 027001 (2023).

Exascale transport simulations for the understanding of the switching mechanism in atomically thin memristors

Liangbo Liang (Oak Ridge National Laboratory); Wenchang Lu; Emil Briggs; Jerzy Bernholc; Panchapakesan Ganesh (Oak Ridge National Laboratory)

Non-volatile resistive switching has emerged as an important concept in the development of high-density information storage and computing. The recent discovery of NVRS in two-dimensional (2D) monolayer structures, such as hexagonal boron nitride (hBN), open a new avenue for ultrathin memory/computing devices. The switching mechanism in 2D monolayers, however, is not fully understood. It is hypothesized that vacancies in 2D monolayers mediate formation of conducting filaments leading to a high- to low resistance state. However, questions remain as to why the current on/off ratio and switching voltage are both strongly device-dependent and vary significantly among different experimental works. To address these questions, it is highly desirable to simulate the electronic transport in a realistic device geometry using ab initio approaches for comparison with experimental data. This is rather challenging as quantum transport simulations are computationally demanding. Here, we report results from simulations of electronic transport of ~1000 atom systems consisting of a hBN monolayer sandwiched by gold electrodes and compute I-V curves. These quantum transport simulations are made possible by implementing the non-equilibrium Green's function method in a highly scalable first-principles DFT code: the Real-space MultiGrid (RMG) that runs efficiently in the first exascale supercomputer, Frontier, at ORNL. Systematic calculations reveal that experimental devices exhibit a wide range of on/off ratios due to variations in interface distances between the electrode and h-BN that significantly modulates the gold/h-BN wavefunction overlap. In addition, DFT calculations demonstrate that the energy barrier of a gold atom to dissociate from the electrode and bind with h-BN increases dramatically with the interface distance, thereby explaining the strong dependence of the switching voltage on distance. Our work provides a deeper understanding of the resistive switching mechanism in atomically thin memristors and demonstrates the significance of interface distance in governing the current on/off ratio and switching voltage.

Using neutron to probe magnetic symmetries of quantum materials

Xianghan Xu (University of Minnesota, Twin Cities)

Symmetries fundamentally govern the emergent collective behaviors in quantum materials. Beyond crystallographic symmetries, magnetic symmetries, which arising from ordered spin configurations, also play a critical role in determining physical properties. Probing the full symmetry landscape, including its evolution under external stimuli, is essential for understanding exotic phases and guiding the design of materials with functionalities. In this talk, I will present my recent work using neutron techniques to resolve nontrivial magnetic textures involving chirality and toroidicity, and to investigate their interplay with electric degrees of freedom, thereby establishing direct links between magnetic space group symmetries and macroscopic physical responses.

Soft matter, polymers, and complex fluids (Tuesday 1:30-4:00 PM)

Complex thermodynamics, structure and dynamics of mixed surfactant “frenemies” on highly curved interfaces

Matthew Helgeson (UC Santa Barbara)

Tanvi Sheth, Andrea Perez, Nairiti Sinha, David Zhao, Glenn Fredrickson, M. Scott Shell and Matthew E. Helgeson

Surfactant mixtures and blends are ubiquitous in industrial practice – yet little is understood about the molecular interactions they experience at fluid interfaces, and how these interactions control interfacial properties. In this talk, we report on the incredible complexity that mixed surfactants can exhibit, and our attempts to use neutrons to understand their interfacial thermodynamics, structure and mechanics to design and stabilize complex emulsion systems. We focus on relatively simple mixtures of surfactant “frenemies” – co-surfactants with homologous chemistry but dissimilar spontaneous curvature. Placing such mixtures on oil-water interfaces with nanoscale curvature (i.e., microemulsions and nanoemulsions) leads to complex vesicular structures, whose phase behavior can be readily tuned through the different spontaneous curvatures of the co-surfactant pair. Using contrast-variation neutron scattering, we demonstrate that the appearance of these structures correlates with interfacial demixing of the co-surfactants. Using a combination of experiments, theory and simulation, we provide a molecular explanation for this behavior, and use it to construct a model for the interfacial thermodynamics that simultaneously predicts the occurrence of demixing and the observed emulsion morphology phase behavior. Finally, we use neutron spin echo to show that these systems exhibit highly non-trivial interfacial mechanics, opening new frontier questions and opportunities to explore how nonideal mixing/demixing and nanoscale curvature can be used to control the mechanics of mixed surfactant interfaces.

Automated Analysis of Time-Dependent Specular Neutron Reflectometry from Thin Films of Polymers Using Neural Networks

Rajeev Kumar (Oak Ridge National Laboratory)

Neutron reflectometry (NR) is a unique characterization technique for studying the structure of thin films due to its high spatial resolution, non-destructive nature, and the sensitivity of neutrons to both isotopes and spin. Machine Learning techniques, on the other hand, provide the opportunity to analyze large amount of data and predict outcomes. Here, we combine machine learning and NR data, both experimental and simulated data, in a series of workflows that enable predicting the structural parameters of thin polymer films from NR data, generating NR curves from Scattering Length Density profiles curves (and vice versa), and predicting the time evolution of NR data. As a toolkit, this set of workflows represent a step forward towards facilitating the analysis, interpretation, and prediction of NR signals, paving the road to automatization. In this talk, I will discuss application of these workflows to thin films of ionic block copolymers in applied electric fields.

Using SANS to characterize how non-adsorbing polymers affect rheology and microstructure of dense suspensions

Akul Seshadri (School of Materials Engineering, Purdue University)

Dense suspensions with high solid volume fractions ($\phi \geq 0.5$) are prevalent in nature and throughout industry. These highly loaded suspensions can exhibit complex rheological behaviors, including both shear thinning and subsequent thickening with increasing shear rate. Understanding the mechanisms behind these rheological behaviors can improve the design of materials systems to behave as predicted and desired under process flows, such as in direct ink writing. Here, we present a study on a dense ($\phi = 0.55$) suspension of colloidal alumina particles and show how the addition and loading of a non-adsorbing polyvinylpyrrolidone (PVP) at different molecular weights can be used to tune and control its rheological properties. PVP was added at varying concentrations spanning the dilute and semi-dilute, non-entangled regimes for each molecular weight. We performed SANS experiments on polymer solutions to obtain relevant equilibrium length scales for each polymer MW at each concentration studied. The addition of PVP at concentrations in the dilute regime was shown to increase the viscosity of the suspension and induce discontinuous shear thickening (DST). However, further increases in PVP loading particularly within the semi-dilute, non-entangled regime and at higher PVP molecular weights also increased the dynamic yield stress of the material, made the suspension more shear thinning, and delayed the onset of DST. We also performed Rheo-SANS measurements on dense polymer-particle suspensions but did not detect any structural changes with shear for either PVP or alumina, which was a surprising finding. Finally, we will present ideas for future Rheo-SANS experiments on more idealized systems which could improve our understanding of how polymeric additives can be used to control the rheological behavior and processing of dense suspensions.

How topological polymer loops on the nanoparticle surface control the mechanical properties of nanocomposites

Tad Koga (Stony Brook University)

Department of Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, New York 11794-2275

Carbon black (CB) and silica (SiO2) filled elastomers are known to be the most successful polymer nanocomposites (PNCs) in industry, where “bound rubber (BR)” (i.e., polymer chains that are physically or chemically adsorbed on the nanofiller surface) plays a critical role in their reinforcement. Here, we report a molecular-scale mechanism underlying the ""BR-induced reinforcement” by integrating neutron scattering experiments and molecular dynamics simulations. Simplified non-crosslinked SiO2-filled polybutadiene (PB) and CB-filled PB reveal the critical role of topological polymer loops in the BR for the enhanced mechanical performance. The average loop size on the SiO2 surface modified with a silane coupling agent is much smaller than that on the CB surface and the loops on the SiO2 surface are densely formed, preventing interdigitation with the matrix chains. On the other hand, the larger, uncrowded loops formed on the CB surface facilitate the interdigitation with the matrix polymer chains even near the filler surface. In this way, a strong connectivity is established between a matrix and a nanofiller, resulting in an adhesive filler-polymer interface. Our findings shed light on rich and complex physics and materials design problems in PNCs, where the topological polymer structure on the nanofiller surface directly controls the macroscopic mechanical properties.

Complexity in the medium-range order as a polyvalent liquid metal

Chengyun Hua (Oak Ridge National Laboratory)

Gallium is a prototypical liquid metal and has gained resurgent attention due to its unique properties. Its atomic dynamics remain elusive despite a large number of studies, mainly due to the challenges of quantifying the atomic-scale dynamics of liquids. Recent developments in inelastic neutron scattering enable us to measure the Van Hove correlation function that describes the real-space motion of liquid atoms. In this work, we use this approach to reveal the dynamics in gallium liquids and find the co-existence of two medium-range orders (MROs), which have a distinct dynamical behavior from that of the short-range order (SRO). We propose that the two types of MRO are strongly overlapping in space and fluctuating in time and are the basis for anomalous behavior of liquid gallium. This view challenges the current view that liquid gallium consists of fluctuating metallic and insulating domains. These findings shed new light on the interpretation of similar microscopic anomalies observed in other semi-metallic liquids.

Neutron Scattering Insights Into Molecular Parameters Governing Hyperuniformity in Brush-Based Hybrid Materials

Michael Bockstaller (Carnegie Mellon University); Jirameth Tarnsangpradit

Disordered hyperuniform (DH) materials represent an ‘exotic’ class of materials that is characterized by the suppression of long-wavelength fluctuations (like single crystals) and the absence of long-range order (like liquids or regular amorphous materials). The concurrence of these otherwise mutually exclusive structure characteristics holds opportunities for the fabrication of heterogeneous materials with novel physical property combinations that could be relevant to a wide range of innovative material technologies. Simulation studies suggest molecular crowding in polymeric systems to favor localization and thus provide a path to realize DH materials.

This contribution will present the application of small angle neutron scattering (SANS) to elucidate the parameters promoting the emergence of disordered hyperuniformity in polymer-grafted nanoparticle (aka particle brush)-based hybrid materials. A unique material system based on hyperbranched polymer nanogel brush particles enables the controlled and independent variation of brush softness and architecture, heterogeneity, the elastic properties of the particle core as well as the neutron scattering length density of core and brush constituents. SANS analysis is used to determine the structure factor of particle brush assembly structures and degree of hyperuniformity of brush particle assembly structures as a function of chain crowding and process parameters. The results reveal 'molecular design guidelines' to realize brush architectures with hyperuniform microstructure and increased inorganic content for enhanced functionality.

AI and Data Science (Tuesday 1:30-4:00 PM)

Case Studies of Machine Learning in Nano and Materials Sciences

De-en Jiang (Vanderbilt University)

What to learn and predict is a question facing domain scientists when they would like to leverage the advances in machine learning to their specific areas of research. In this talk, I will discuss how my group is answering this question in my research interest of computational materials chemistry for nanocatalysis and energy storage. Through two case studies, I will show the power of deep neural networks in locating hydrides in copper nanoparticles (highly relevant to neutron scattering) and machine learning potentials in understanding superionic Li transport in amorphous materials. I hope to convince you that machine learning is now a key approach in predictive modeling in nano and materials sciences.

Recent AI projects for neutron data analysis and automation at SNS

Mathieu Doucet (Oak Ridge National Laboratory)

The field of Artificial Intelligence (AI) is experiencing a period of rapid growth, bringing transformative changes to many scientific domains. This presentation will provide a brief overview of the evolution of AI, highlighting key milestones and their relevance to neutron scattering. We will review the progression of our work, from early applications of neural networks to more recent developments using transformers for data analysis in techniques like reflectometry, SANS, and diffraction. We will then discuss our current focus on agentic AI and the development of automated workflows to enable on-the-fly experiment steering and more efficient data interpretation.

Unsupervised Subspace Decomposition for Fast Hyperspectral Neutron Tomography

Samin Chowdhury (Purdue University)

Hyperspectral Neutron Computed Tomography (HSnCT) is an advanced imaging technique in which thousands of wavelength-resolved neutron radiographs are acquired for each tomographic view. Traditionally, hyperspectral reconstruction is performed by reconstructing each neutron wavelength bin separately, which is extremely time-consuming and often produces low-quality reconstructions due to low signal-to-noise ratios. Consequently, material decomposition based on these reconstructions tends to produce erroneous volumetric material separation and inaccurate estimates of the material spectra.

To address these challenges, we introduce two novel algorithms: Fast Hyperspectral Reconstruction (FHR) and Fast Material Decomposition (FMD).

- FHR is a method for fast tomographic reconstruction of hyperspectral data that also visibly and quantitatively reduces noise and improves reconstruction quality.
- FMD is a related method to perform material decomposition, producing 3D reconstructions of component materials and the associated linear attenuation coefficient spectra.

Figure 1 illustrates the core components of FHR and FMD. Both algorithms are based on an unsupervised subspace decomposition procedure that represents the high-dimensional hyperspectral views within a low-dimensional intermediate subspace. The subspace components are then reconstructed using model-based iterative reconstruction (MBIR). The FHR algorithm then directly expands the subspace reconstructions to obtain the hyperspectral reconstructions. Alternatively, the FMD algorithm then volumetrically decomposes the object's materials from the subspace reconstructions and produces the 3D reconstructions of individual materials and their associated spectra. The use of subspace decomposition in our algorithms serves three purposes:

- Eliminates significant spectral noise from data while fitting into low-dimensional subspace.
- Enables over 10x faster computation due to the reduced number of tomographic reconstructions.
- Allows the use of (MBIR) that produces high-quality reconstructions from sparse view data.

We apply our algorithms to simulated and measured neutron data and demonstrate that they are substantially faster and yield more accurate results than traditional HSnCT methods. A comprehensive description of this work is provided in our recent publication [1].

References

[1] M. S. N. Chowdhury et al., ""Fast Hyperspectral Neutron Tomography,"" in IEEE Transactions on Computational Imaging, vol. 11, pp. 663-677, 2025, doi: 10.1109/TCI.2025.3567854.

AI enabled modeling of correlated quantum matter

Thomas Maier (Oak Ridge National Laboratory)

Strongly correlated quantum materials promise to revolutionize many energy-related technologies, but owing to their complexity, their discovery process is rather slow. This talk will discuss how AI can help speed up this process: By accelerating expensive computational simulations and facilitating the conversion of abstract numerical data into experimentally accessible observables, AI can enable a tight integration between simulations and experiments, and thus significantly accelerate the quantum materials discovery process. This vision and proof-of-concept results will be demonstrated for ORNL’s DCA++ research code, a quantum Monte Carlo application for advanced high-performance computing-based simulations of correlated quantum materials.

An Extreme-Scale Multi-Fidelity Computational Active Learning Paradigm Towards Realizing Autonomous Synthesis

Panchapakesan Ganesh (Oak Ridge National Laboratory); Soumendu Bagchi (Oak Ridge National Laboratory); Ryan Morelock (Oak Ridge National Lab); Addis Fuhr; Ayana Ghosh (Oak Ridge National Laboratory); Debangshu Mukherjee; Thomas Maier

Traditional approaches to bridge atomistic dynamics with experimental observations at the microstructural level often rely on phenomenological models of the underlying physics, whose free parameters are in turn fitted to a small number of intuition-driven atomic scale simulations under limited number of thermodynamical drivers (e.g., temperature, pressure, chemical potential etc). This tedious and time-consuming approach becomes particularly cumbersome to study synthesis of chemicals and materials with complex dependencies on local environment, temperature and lattice-strains e.g., heterostructure interfaces of nanomaterials. In this talk, I will present workflows that couple automated exascale high-throughput large-scale DFT calculations, ensemble force-field fitting and molecular dynamics simulations with a wide range of uncertainty quantification-driven active learning paradigms for on-the-fly learning of material synthesis trajectories, to create an autonomous computational synthesis platform. By implementing such a workflow to study recrystallization of amorphous transition-metal dichalcogenide (TMDC) phases under various growth parameters, I will show that such automated multi-fidelity frameworks can be promising towards achieving controlled epitaxy of targeted multilayer moiré devices paving the way towards a robust autonoumous discovery pipeline to enable unprecedented functionalities. Opportunities to use these autonomous computational synthesis pipelines to create 'digital twins' of synthesis trajectories, train generative inverse-design machine-learning algorithms to predict new materials and their synthesis parameters with targeted properties, and eventually accelarate experimental synthesis will also be presented.

Enabling Autonomous Labs: The NSDF-ORNL Partnership for Real-Time Scientific Discovery

Michela Taufer (University of Tennessee Knoxville)

Autonomous labs are transforming scientific discovery by combining experimental steering, AI at the edge, real-time data movement, and in-situ decision making. Recent advances in these individual domains have made autonomous labs possible; however, the next major challenge is to break down disciplinary silos and build integrated ecosystems that make autonomous science accessible, scalable, and sustainable.

This talk highlights the successful collaboration between the National Science Data Fabric (NSDF) and the INTERSECT initiative at Oak Ridge National Laboratory (ORNL), advancing real-time monitoring and steering of autonomous experiments. We present a modular, multi-service architecture integrating NSDF capabilities for message processing, live visualization dashboards, and persistent cloud storage. These services are actively deployed at ORNL and CHESS, supporting autonomous neutron diffraction, quantum materials workflows, flow chemistry, smart manufacturing, and energy systems. Designed for portability and scalability, NSDF's containerized, Kubernetes-orchestrated infrastructure enables FAIR, AI-ready workflows that empower domain scientists, foster interdisciplinary research, and accelerate discovery through reusable and shareable data systems.

Wednesday Plenary Session

Characterizing Materials and Interfaces in Solid-State Batteries

Matthew McDowell (Georgia Tech)

Matthew T. McDowell
Professor and Carter N. Paden, Jr. Distinguished Chair
G. W. Woodruff School of Mechanical Engineering
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Georgia Institute of Technology, USA

The advent of lithium-ion batteries has brought about a revolution in portable energy storage, spurring the rapid growth of the electric vehicle market. However, further advances in energy storage technologies are needed for electric trucks and planes, as well as for grid storage. Here, I will discuss my group's research on solid-state batteries, which is a rapidly developing technology that could feature higher energy density and improved safety compared to lithium-ion batteries. The presence of solid-solid electrochemical interfaces within solid-state batteries, rather than conventional liquid-solid interfaces, causes different fundamental phenomena to govern behavior of these batteries. Using operando X-ray tomography, cryo-FIB, and other characterization techniques, we visualize the formation of voids during lithium stripping and dendrite growth during plating. Next, alloy anodes are shown to exhibit improved interfacial stability and enhanced cyclability in solid-state batteries compared to Li-ion batteries. The influence of stack pressure on alloy anode evolution is investigated, and we show that anode morphology changes during charge/discharge are highly pressure dependent. Finally, I will briefly discuss other energy storage innovations, including battery materials with improved sustainability and new battery concepts for ultrahigh energy density. Taken together, knowledge of transformation mechanisms in materials is key for engineering them for improved performance, with new materials holding great promise for future battery technologies."

From Phase Separation to Vaccine Design: Small-Angle Scattering in Biomolecular Research

Amy Xu (Louisiana State University)

Neutron scattering is a powerful characterization technique for investigating the structure and dynamics of biomacromolecules, as well as their interactions. In particular, small-angle neutron scattering (SANS) enables the characterization of structural features across a wide range of length scales, from just a few nanometers to several hundred nanometers. Additionally, SANS offers unique advantages through contrast matching, allowing for the selective characterization of individual components within complex structures and providing insights into the hydration states of the measured materials. Our research utilizes neutron scattering to investigate biomacromolecular interactions with the primary objective of gaining a deeper understanding of their biological functions and material properties. Our research extends in two major directions: (1) understanding the phase behavior of biomacromolecular complexes in various crowded environments, as recent studies highlight the importance of liquid-liquid phase separation (LLPS) in underpinning fundamental biological processes, and (2) elucidating the mechanism of action of aluminum adjuvants in vaccine formulations. By employing SANS, we have probed the hydration and porosity of aluminum adjuvants, providing critical insights into their microstructures. These studies yield critical insights into the microstructures of aluminum adjuvants and offer new perspectives on their functional mechanisms. Together, these studies highlight the power of neutron scattering in providing fundamental, molecular-level insights into biomacromolecular interactions—knowledge that can inform both basic biological research and the rational design of functional materials across diverse fields."

Hard matter 2: Energy materials (Wednesday 1:30-3:30 PM)

Understanding static and dynamic local structure in Hybrid Metal Halide Perovskites

Michael Toney (University of Colorado Boulder)

Local atomic structure often differs from the global average structure as measured with diffraction and yet the local structure has a profound impact on materials functionalities. This structure-function relationship applies in many materials classes, ranging from organics to Li-ion battery cathodes to oxide and halide perovskites. Accurately characterizing this local structure has proven challenging but recent advances in neutron and X-ray diffuse scattering ("between" Bragg peaks) has enabled local structure determination.

In this talk, I will discuss the importance of local structure and how this can be quantified and will demonstrate this for organic-inorganic hybrid halide perovskites [1,2]. These materials are a recently re-invigorated class of semiconductors that have demonstrated very high efficiencies for solar cells after just over a decade of research. While the importance of lattice dynamics and dynamical (dis)order have been recognized in these materials, their nature is only poorly known and understood. We used X-ray and neutron diffuse scattering coupled with molecular dynamics to quantify the nature, size, and time scale associated with dynamical local order in CH3NH3PbI3 and CH3NH3PbBr3 perovskites. We observe that the nominally cubic perovskite consists of dynamical, two-dimensional sheets of lower symmetry tetragonal regions of about 3 nm diameter with several picosecond lifetimes. The implications for halide perovskite optoelectronic properties will be discussed.

[1] NJ Weadock et al., Joule 7, 5, 1051-1066 (2023)
[2] DM Ladd, unpublished.

Quasi-Elastic Neutron Scattering for Investigating Dynamic Behavior in Energy Materials

Naresh Osti (Oak Ridge National Laboratory | SNS | HFIR)

Understanding the microscopic dynamics of various constituents in energy materials is crucial for exploring the fundamental mechanisms of energy storage and plays a significant role in their applications within energy storage and conversion technologies. By acquiring molecular-level structural and dynamic information about electrodes and electrolytes, we can create new materials with enhanced properties that lead to better performance in device applications. In this study, we present dynamic investigations of different energy materials, including 2D-layered transition metal carbides, as well as solid-state lithium and polymer electrolytes. We will discuss the stochastic dynamics—originating from both diffusive and relaxational processes—in the picosecond to nanosecond time range, as revealed by quasielastic neutron scattering and simulations.

Atomically Dispersed Metal sites for Electrochemical Energy Conversion

Gang Wu (Washington University in St. Louis)

This abstract focuses on the recent work in developing the most promising PGM-free catalysts for electrochemical energy applications, which are closed collaborated with scientists at Oak Ridge National lab. In particular, single and dual atom catalysts based on atomically dispersed, nitrogen-coordinated metal sites (M–N–C catalysts) will be discussed in terms of their history, present achievements, and remaining challenges. We specifically concentrate on the active-site structure and critical factors governing catalytic activity and performance durability for various critical electrochemical reactions, including oxygen reduction and CO2 reduction, for energy storage and conversion. We highlighted potentially effective strategies for improving performance by controlling the catalyst structure at the atomic scale, mesoscale, and nanoscale. We discuss the importance of overcoming often-observed activity–stability trade-offs and the importance of advanced modelling for the rational design of catalysts.

Creating new THz Photodetectors with Topological Semimetals

David Mandrus (University of Tennessee)

Recent advances in understanding Berry curvature effects have shown that the topological properties and electronic band structure of noncentrosymmetric semimetals can be harnessed to achieve quantum-limit THz detection, overcoming traditional limitations through giant nonlinear optoelectronic and optical effects. These breakthroughs open new pathways for quantum THz sensing, light sources, and frequency transduction applications. In this talk I will discuss the theoretical background and experimental progress made so far toward realizing these quantum devices."

Scalable Bottom-Up Synthesis of Nanoporous Hexagonal Boron Nitride (h-BN) for Large-Area Atomically Thin Ceramic Membranes

Piran Kidambi (Vanderbilt University)

Nanopores embedded within monolayer hexagonal boron nitride (h-BN) offer possibilities of creating atomically thin ceramic membranes with unique combinations of high permeance (atomic thinness), high selectivity (via molecular sieving), increased thermal stability, and superior chemical resistance. However, fabricating size-selective nanopores in monolayer h-BN via scalable top-down processes remains nontrivial due to its chemical inertness, and characterizing nanopore size distribution over a large area remains extremely challenging. Here, we demonstrate a facile and scalable approach of exploiting the chemical vapor deposition (CVD) process temperature to enable direct incorporation of subnanometer/nanoscale pores into the monolayer h-BN lattice, in combination with manufacturing compatible polymer casting to fabricate centimeter-scale nanoporous atomically thin ceramic membranes. We leverage diffusive transport of analytes including size-selective Ficoll sieving to characterize subnanometer-scale and nanoscale defects that manifest as pores in centimeter-scale h-BN membranes, overcoming previous limitations in large-area characterization of nanoscale defects in h-BN. Our approach opens a new frontier to advance atomically thin membranes to 2D ceramic materials, such as h-BN via facile and direct formation of nanopores, for size-selective separations.

References:
Naclerio et al. Nano Letters 2025
Naclerio et al. Adv. Mat. 2024
Kidambi et al. Chem. Mat. 2014

Biology and Life Sciences (Wednesday 1:30-3:30 PM)

Advances in automated sample preparation for neutron reflectometry experiments

David Hoogerheide (NIST Center for Neutron Research)

Neutron reflectometry is a powerful tool for interrogating the structure of thin films at interfaces. Surface-adsorbed lipid bilayers in liquid flow cells provide a platform for a wide range of biophysical measurements, from protein structures to antimicrobial peptide activity to interfacial forces. Lipid bilayers are chemically complex, with an enormous combinatorial space of compositions; as a result, bilayers of arbitrary lipid compositions cannot always be formed using conventional methods. A compounding factor is the even larger combinatorial space of protein or peptide binding partners. These factors conspire to significantly limit the scope of neutron reflectometry measurements relative to that required to answer the broadest biophysical questions and aid biotechnological development. In this talk, I will describe how sample environment developments at LIQREF have enabled progress towards automated lipid bilayer formation of a broad range of lipid compositions on various substrate chemistries. I will report on the formation of stable surface-adsorbed bilayers comprising primarily non-lamellar lipids such as those common in bacterial and mitochondrial membranes. Finally, I will introduce the NIST ROADMAP project for neutron reflectometry-driven autonomous discovery of membrane-active peptides and present results demonstrating how autonomous experimentation can drive increased measurement throughput in this space.

Shining light (and neutrons) on RNAs

Sarah Keane (University of Michigan)

The structures of RNAs and RNA-containing complexes regulate many biological processes. Despite their functional importance, RNA:RNA complexes represent a small fraction of experimentally-determined structures. We employed a joint small-angle X-ray and neutron scattering (SAXS/SANS) approach to structurally interrogate conformational changes in a model RNA:RNA complex. Using a combination of isotope labeling and contrast matching (CM), we were able to probe the bound state structure of an RNA within a selectively deuterated RNA:RNA complex, expanding the utility of SANS for complex structure elucidation. This work demonstrates that in silico modeling, SAXS, and CM-SANS can be used in concert to directly analyze conformational changes within RNAs when in complex, enhancing our understanding of RNA structure in functional assemblies.

The role of non-equilibrium ribosomal dynamics in facilitating nucleoid separation

Chathuddasie Amarasinghe (University of Tennessee, Knoxville); Mu-Hung Chang (University of Tennessee); Jaana Mannik;
Scott Retterer (CNMS); Maxim Lavrentovich; Jaan Mannik

The molecular mechanism of how the two sister chromosomes segregate and partition to two daughter cells in bacteria is not yet understood. A recent theoretical model has proposed that out-of-equilibrium processes associated with ribosome-mRNA (polysome) dynamics significantly influence the segregation of the two chromosomes. Here, we investigate the role of ribosomal dynamics on nucleoid separation using high throughput fluorescence microscopy in microfluidic devices and compare experimental results to our own reaction-diffusion model of ribosome subunits, polysomes and chromosomal DNA. Our experiments reveal that while non-equilibrium dynamics drives ribosomes to the mid-cell, as predicted by the model, the effect associated with these dynamics appears to have a much weaker effect on the segregation than predicted by the model. Instead, our data suggest that the closing division septum via steric interactions and potentially entropic forces between two DNA strands coupled to cell elongation promote partitioning of the nucleoids to two daughter cells.

Nanostructured Silicon Optical Biosensors: From On-Chip to Paper-Based Diagnostics

Sharon Weiss (Vanderbilt University)

Silicon-based optical structures such as interferometers, ring resonators, and photonic crystals hold great promise as low-cost sensor elements in part due to their compatibility with both standard microelectronics processing and standard surface functionalization techniques. The sensitivity of silicon-based optical biosensors is derived from the level of interaction between light and the target molecules to be detected as well as the ability of the sensor to selectively and robustly capture the desired target molecules. This talk will discuss (1) approaches to increase the detection sensitivity of on-chip optical biosensors through the use of subwavelength engineering to increase the light-molecule interaction and (2) the realization of nanoscale porous silicon membrane interferometers on paper-based supports as a new platform for quantitative rapid diagnostic tests with optical readout.

Pyrvinium Pamoate's Effect on Models Lipid Membranes.

Zuzanna Kulik (Division of Translational Oncology, Intercollegiate Faculty of Biotechnology, University of Gdańsk and Medical University of Gdańsk, Gdańsk, Poland.)

Pyrvinium is a fluorescent red cyanine dye, whose salts - pyrvinium chloride salt and pyrvinium pamoate (PP) - have been extensively researched in a wide range of conditions. It has been approved by the FDA as a treatment for pinworm infestations. The substance's anti-cancer potential has garnered increasing attention in recent years and first clinical trial on the use of PP to treat pancreatic cancer has recently been launched.

We present the first results on the effect of PP on a model membrane using neutron scattering. As a model system, simple 1-palmitoyl-2-oleoyl-glycero-3-phosphocholine (POPC) lipid bilayer was used with varying concentration of cholesterol, and we performed small angle neutron scattering (SANS) and neutron spin echo (NSE) experiments. Our results indicate that while PP does not significantly change the structure of a lipid bilayer, it changes the mechanical properties of a membrane, and the effect varies with PP concentration. These results provide molecular level insights of the interaction of PP with lipid membranes.

Emerging Research and Multimodal Techniques (Wednesday 1:30-3:30 PM)

Patterning Defects in Aluminum Nitride for Ferroelectrics and Integrated Photonics

Bogdan Dryzhakov (Oak Ridge National Laboratory)

TBD

Nanoscale Structure of Lithium-ion Battery Cathodes Probed Using Contrast Variation Neutron Scattering

Jeffrey Richards (Northwestern University)

Understanding the link between how porous lithium-ion battery (LIB) electrodes are manufactured and the structure-function relationships that determine their performance is critical to accelerating the development of emergent battery technologies with higher rate cycling and capacity. Porous electrodes are manufactured by suspending a mixture of micron-sized electrochemically active material, polymer binder, and carbon black (CB) in a solvent and depositing it onto a metallic current collector. The complex processing conditions encountered during formulation and coating create many challenges for developing quantitative structure-property relationships. Neutron scattering measurements, performed through collaborations at National Laboratories, are essential to discovering these relationships and exploiting them for lithium-ion battery design. In this talk, I will describe our group's collaboration with Oak Ridge National Laboratory to develop unique sample environments and analysis methods for neutron scattering measurements applied to battery science. In particular, I will focus on the use of contrast variation to elucidate the nano- and micro- scale interphases within the porous electrode.

Unveiling Magnetic Excitations in Low-Dimensional Mn-Doped II–VI Semiconductors

Yi-Hsin Liu (National Taiwan Normal University)

This presentation explores the quantum spin dynamics and magnetic exchange interactions in Mn-doped II–VI semiconductor nanostructures—specifically $(Cd_{1-x}Mn_xSe)_{13}$ nanoclusters and monolayer $ZnSe(en)_{0.5}$—using both optical and neutron-based techniques. These hybrid materials exhibit rich spin-dependent phenomena, including giant Zeeman splitting, exciton–magnon coupling, and magnetic polaron formation, driven by strong sp–d exchange interactions and spin–orbit coupling (SOC) in reduced dimensions. Time-resolved photoluminescence (PL) and magneto-circular dichroism (MCD) measurements confirm spin-polarized excitonic states and magnetic field-tunable photophysics.

To go beyond surface-level magnetometry, we propose a comprehensive inelastic neutron scattering (INS) study—leveraging instruments such as Pelican, SEQUOIA, and ARCS—to directly probe low-energy spin-wave excitations, resolve momentum-dependent spin dispersion, and extract magnetic exchange constants via linear spin-wave theory. Measurements across doping concentrations (0.5–15%), temperatures (2–300 K), and magnetic fields (up to 3 T) will enable mapping of spin fluctuation spectra and exciton–magnon resonances. The use of polarized neutron analysis will isolate magnetic contributions from nuclear background, offering enhanced sensitivity to weak spin excitations in layered materials.

Complementary structural validation by XRD ensures phase purity, while the observed anomalous Bohr magnetons and ligand-dependent spin responses in nanoclusters underscore the importance of chemical control. Collectively, this research establishes a foundational pathway to engineer spin coherence and quantum photonic functionalities in 2D and 0D semiconductors using neutron spectroscopy.

(Dis)order in the court: Probing Imperfections in Quantum Materials with Monochromated EELS

Kory Burns (University of Virginia)

Kory Burns1, Eva Zarkadoula2, Chris Smyth3, Jordan A. Hachtel2

Two-dimensional (2D) compound semiconductors and dielectrics exhibit a range of levels of disorder dependent on their stoichiometry, which can be engineered based on growth conditions, substrate interactions, or atom-by-atom modifications with charged projectiles. There is an entire framework of studies that builds upon research dedicated towards the associated properties with heterogeneities in films, but fail to make one-to-one correlations with the atomic arrangement of the lattice and the optical/infrared emissions. In this talk, we first use aberration-corrected scanning transmission electron microscopy (STEM) to visualize the atomic sites, then machine learning to map out the positions and relative displacement of the atoms in the vicinity of defects. Next, core-loss electron energy loss spectroscopy (EELS) is used to determine the global and local composition, as well as localized carbon and oxygen impurities to unveil their role in stabilizing strain-driven polymorph. Last, monochromated EELS inside an aberration-corrected STEM is used, which greatly reduces the energy distribution of the electron source to maximize the energy resolution without sacrificing too much spatial resolution. Accordingly, we map the high-frequency vibrational modes and exciton complexes in transition metal dichalcogenides (TMDs) and barrier layers in Josephson junctions using off-axis EELS to correlate the impact single-atom modifications have on the vibrational and optical spectrum. Ultimately, we address applications ranging from quantum sensors to thermoelectric junction devices.

References:

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Imaging of AFSD Al 6061 and a 6061-TiN MMC

Bernadette Cladek (University of Tennessee Knoxville)

Additive friction stir deposition (AFSD) is a rapidly developing additive manufacturing (AM) process which is derived from friction stir welding (FSW). Unlike fusion-based AM methods which involve melting, AFSD is a solid state process which relies on heat generated during plastic deformation, reaching 60-90% of the deposited material's melting temperature. Solid state processes avoid problems encountered during solidification, can utilize commercially available feedstock, and can build parts at a higher rate and larger scale than fusion-based AM. However, AFSD equipment has only become commercially available within the last 5-6 years, and the challenges for industrial utilization of AFSD are still being discovered. Feedstock composition, toolhead rotation speed, deposition track (direction and travel speed), and the resulting temperature distribution affect plasticity of the deposit, and consequently microstructure development and texture in the printed part. This can result in bulk heterogeneity and anisotropy of mechanical properties in the printed part. This work explores structural heterogeneity in AFSD alloys and metal matrix composites (MMCs) printed with this new AM technology, which varies over micrometer to centimeter length scales along the build directions of the deposition. We are investigating processing-structure-property-performance relationships, aiming to correlate microstructure and mechanical property variations throughout the layers of the build. The penetration depth of neutron imaging, paired contrasting lubricant and composite particles, will indicate how these secondary phases are distributed by friction stir process at a length scale commensurate with part size. These results demonstrate successful use of neutron imaging and computed tomography to quantitatively analyze composite particle mixing through a bulk part. Understanding interlayer mixing behavior with and without a composite particle in AFSD Al6061will lead to better understanding of material flow, plasticity, and recrystallization behavior during deposition.