

CENTER FOR NANOPHASE MATERIALS SCIENCES

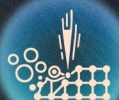
SCIENTIFIC STRATEGIC PLAN
FY25-30



UNDERSTAND & UTILIZE
HETEROGENEITIES IN
QUANTUM MATERIALS



HARNESS COMPLEX
MACROMOLECULAR
CONFORMATIONS



DIRECT MULTISCALE
DYNAMICS &
TRANSFORMATIONS

LEAD IN AUTONOMOUS
& DATA-DRIVEN
NANOSCIENCE



STRENGTHEN
INTEGRATION INTO THE
NATIONAL USER FACILITY
ECOSYSTEM



FOSTER A THRIVING
USER COMMUNITY &
STAFF DEVELOPMENT



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Executive Summary

This strategic plan for the U.S. Department of Energy’s Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) defines a vision centered on accelerating materials discovery in close collaboration with our user community and partner facilities. CNMS will achieve this by integrating deep scientific knowledge with one-of-a-kind synthesis, characterization, and modeling capabilities, leveraging autonomous experimentation and AI/ML to connect these elements into a seamless, human-centered discovery loop that expands what can be explored, understood, and designed at the nanoscale. As one of the five U.S. Department of Energy (DOE) Nanoscale Science Research Centers (NSRCs), CNMS is uniquely positioned to advance this vision by combining its breadth of scientific capabilities with a user-accessible, GPU-enabled cloud environment that supports real-time data analysis, AI/ML model development, and scalable computational workflows. This infrastructure enables the rapid generation, curation, and exploitation of rich, high-quality multimodal datasets, amplifying researchers’ ability to move efficiently from fundamental insight to application-relevant understanding. Working closely with users and partners across DOE’s Office of Science Scientific User Facilities (SUF) Division ecosystem, CNMS will help address materials challenges central to national priorities in energy innovation, next-generation computing, and energy security while providing rich, high-value datasets critical to supporting the DOE Genesis Mission.

The ability to understand and control materials across the nanoscale plays a foundational role in many of today’s most pressing and emerging scientific challenges. By bridging “atoms to applications,” nanoscience connects fundamental processes such as energy transport, conversion, and structural evolution to the properties and performance of functional materials and devices. These relationships underpin progress in computing, quantum information science, microelectronics, hybrid and soft-hard interfaces, and functional materials. In this strategic plan, CNMS aligns its expertise, capabilities, outreach, and operations around six strategic goals that focus the center’s unique strengths and guide future investments, transforming how we pursue discovery and equipping CNMS to tackle the materials challenges of the coming decade and beyond.

These strategic goals establish a clear framework for advancing CNMS’s multidisciplinary research and scientific priorities, driving the development of next-generation capabilities and deepening the integration of AI/ML, theory, and experiment across the center. They also guide targeted investments and strengthen the collaborative culture that enables CNMS to support its users and staff. The integration of staff science theme research with active support of a vibrant and innovative user program is a key strength of the center. Together, these efforts position CNMS to deliver transformational science, expand its role within the national user facility ecosystem, and advance the frontiers of nanoscience.

As our foremost strategic priority, Goal 1 of the strategic plan orients CNMS to lead in the advancement of AI/ML-enabled autonomous workflows and building customized instrumentation that redefines how nanoscience is conducted. As a foundation for continuing to drive materials discovery through seamless integration of synthesis, characterization, and modeling, the center is

expanding its leading data and digital infrastructure to enhance human-centered autonomy, accelerate the generation of high-quality datasets, and customize the tools available to staff and users. CNMS has rapidly built momentum and leadership in this area through the establishment of the Data NanoAnalytics (DNA) Group, which catalyzes the integration of AI-driven methods across the center. By upskilling domain experts and embedding AI/ML capabilities directly within scientific groups, DNA has become central to *how* CNMS conducts multidisciplinary research, providing the connective tissue that links multimodal measurements across time and length scales and enabling new modes of discovery.

This multidisciplinary work is central to the CNMS's dual mission of advancing world-leading science while supporting a dynamic and impactful user program. By integrating diverse capabilities and deep domain expertise, CNMS addresses scientific challenges that cannot be met by smaller or more narrowly focused research efforts. The center's strength is anchored in eight research groups that maintain state-of-the-art instrumentation and disciplinary excellence across synthesis, characterization, theory, and data analytics. The work of these groups is realized through three cross-cutting scientific themes: Heterogeneities in Quantum Materials (HQM), Harnessing Complex Macromolecular Conformations (HCMC), and Multiscale Dynamics (MD). These themes integrate capabilities across all eight groups to pursue frontier scientific questions and enable cohesive, multidisciplinary workflows. Three of the center's strategic goals (Goals 2-4) are directly shaped by the scientific priorities embodied in these themes, ensuring clear alignment between CNMS's scientific direction, user program, its long-term strategic objectives, and national priorities. Together, this organizational structure ensures that CNMS can sustain high-impact user operations while advancing bold, forward-looking science that contributes to DOE's broader mission in materials discovery and innovation.

Our fifth strategic goal acknowledges that integration within DOE's broader user facility ecosystem is central to the continued success of CNMS. Building on the 90-Day Response to the 2024 BES Operations Review (Appendix C), CNMS has established a detailed roadmap to deepen collaboration with ORNL's Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR). This includes expanding coordinated deuteration and isotopic substitution capabilities, developing integrated characterization and multimodal experimental workflows, and establishing a joint Theory–Modeling–AI/ML Hub. In parallel, coordinated efforts with the other NSRCs focus on sharing autonomous research workflows and standardizing user access processes to enable seamless cross-facility research. Collectively, these initiatives position CNMS with other SUF Division facilities as a source of large, multi-modal, high-quality experimental datasets and digital twins that can be leveraged by the DOE Genesis platform and the broader scientific community.

CNMS recognizes that a successful user program begins with a supported and engaged staff that is committed to both scientific and operational excellence. Strategic Goal 6 focuses on empowering staff by creating opportunities to strengthen communication, streamline user interactions, and enhance professional development across different stages of career development. These efforts—coupled with new mentoring programs, early-career development and onboarding strategies, as well as expanded upskilling for cross-facility engagement—will ensure that CNMS staff continue to

deliver exceptional science and user support while building the workforce needed to support this strategy.

Sustaining excellence requires disciplined investment, risk management, and continuous renewal of infrastructure. CNMS will be guided by a philosophy of dual-value investments, prioritizing those that simultaneously enhance user access and advance emerging science. A continued focus on in-house development of unique instruments co-designed with AI/ML workflows and data infrastructure in mind will facilitate cultivation of unique capabilities that fully integrate with our shared vision on ‘how’ science will be done. Staff hiring, capital and equipment investments, and infrastructure development are all taken into consideration and prioritized as part of a continuous risk-review process. The CNMS continuously updates operational best practices and prioritizes investments based on impact to safety, user continuity, and scientific productivity. Planned recapitalization, proactive maintenance, and strategic workforce development ensure that CNMS remains a consistently high-performing user facility positioned for long-term success.

Through this strategic plan, CNMS affirms its role as a uniquely capable national user facility, one where foundational materials science, one-of-a-kind experimental platforms, and AI-enabled discovery converge to accelerate insight in ways not achievable elsewhere. By uniting deep scientific talent with integrated synthesis, characterization, modeling, and a user-accessible GPU-enabled cloud environment, CNMS offers researchers an end-to-end discovery platform that shortens the path from fundamental understanding to impactful outcomes. Providing a combination of rich multimodal data, autonomous and human-centered workflows, and seamless connection to partner facilities across the DOE ecosystem, CNMS positions itself as a destination facility for tackling the nation’s most challenging materials problems. In doing so, CNMS delivers exceptional user value and a national capability that advances energy innovation, next-generation computing, and security-relevant technologies at the frontiers of nanoscience.

Mission and Vision

Mission

CNMS empowers discovery at the frontiers of nanoscience and materials research by delivering world-leading capabilities, expertise, and workflows that seamlessly integrate synthesis, characterization, modeling, and fabrication. Through its collaborative user program and scientific themes, CNMS drives fundamental discovery that links evolving material structure to function and works with partners to translate these discoveries into technological advances that strengthen the nation's energy future and scientific leadership.

Vision

CNMS will be a leader in the exploration, discovery, and control of complex materials systems through autonomous, data-driven nanoscience that integrates human expertise with advanced, one-of-a-kind analytical and computational tools. By harnessing the unique convergence of world-class synthesis, characterization, and modeling capabilities, CNMS will accelerate fundamental insight and enable translation of discoveries into emerging technologies. Through this combination of deep domain knowledge, innovative experimental platforms, and AI/ML-enabled discovery, CNMS will empower its user community to generate and interpret rich multimodal datasets that push the frontiers of materials science in ways not previously possible.

Path Forward

CNMS will lead pioneering research across its scientific themes, advancing understanding of quantum phenomena, predictive behavior of soft matter, and the multiscale dynamics that drive energy transport and structural evolution in complex material systems. These efforts will reveal how function emerges from the atomic to the nanoscale and how energy transport drives transformations during synthesis, integration, and use. Integrating these themes with data-driven and autonomous methods will position CNMS as a focal point for multidisciplinary discovery and enable progress in creating critical technologies such as quantum information systems, adaptive materials, and next-generation microelectronics.

As a critical member of DOE's Office of Science SUF Division ecosystem, CNMS will collaborate with other NSRCs and light and neutron sources, to develop shared platforms, interoperable data infrastructures, and coordinated workflows that amplify the national impact of nanoscale science. New efforts to empower CNMS staff will enable them to even more deeply engage with users, fostering a culture of collaboration that exceeds expectations and strengthens scientific outcomes. This human-centered approach to autonomous discovery and operational excellence will enhance the CNMS user program, drive cross-facility innovation, and accelerate progress toward a predictive understanding of materials central to the nation's energy, economic, and security priorities.

Introduction: Nanoscience and CNMS

The true promise of nanoscience extends beyond working at a particular length scale. It lies in the nanoscale's role as the bridge between quantum and atomic building blocks and the emergent functional properties that underpin critical technologies. Future opportunities depend not only on accelerating the discovery of new materials and understanding how phenomena emerge across the nanoscale but also on developing a deeper picture of how materials evolve during synthesis, how they transform when integrated into devices, and how they operate and adapt within real-world environments.

As global energy demands grow, society faces a pressing need to improve the efficiency of information processing while advancing materials for next-generation energy conversion, storage, and chemical processes. Breakthroughs in quantum and neuromorphic computing, catalysis, hybrid polymers, and other nanoscale technologies all rely on the ability to synthesize, manipulate, and interrogate materials with exceptional precision and to understand how structure, defects, interfaces, and dynamic processes govern function across multiple scales.

The growing power of AI and high-performance computing, while driving increased demand for advanced materials and more efficient energy use, is simultaneously reshaping how science is conducted, enabling predictive design, automated experimentation, and multiscale simulations that directly address these challenges. Together, these advances are bringing us closer to creating, with atomic precision, the structures envisioned through theory and modeling and to visualizing and predicting their behavior at the level of individual atoms. These scientific and technological advances are reshaping what is possible in nanoscale research, giving us the ability to design materials with atomic-level precision, interrogate their behavior across vast temporal and spatial scales, and connect theory, modeling, and experiment in ways that were previously unimaginable.

The CNMS's six strategic goals reflect this new reality, forming the pillars that guide how the CNMS, as a steward of national nanoscience capabilities and a DOE Office of Science user facility, will transform the practice of nanoscience, lead in frontier theme research areas, and collaboratively expand impact across the DOE mission space.

The remainder of this document outlines how CNMS translates strategic intent into action. Following this introduction, the CNMS strategic goals and high-level objectives are presented to define the center's priorities and desired outcomes. The Implementation and Investment Strategy describes the coordinated actions and capability development needed to advance each goal, including the strategic realignment of the CNMS scientific themes with Strategic Goals 2–4. The document then details investment priorities, risk identification and mitigation approaches, performance metrics, and review and reporting mechanisms, providing a clear framework for execution, assessment, and continuous improvement.

Strategic Goals and Objectives

At its essence, the CNMS vision recognizes and aggressively pursues the opportunity to continue transforming how science is done, embracing autonomous, data-driven, and human-centered approaches that capitalize on deep domain expertise and the development of one-of-a-kind experimental platforms, detectors, tools, and models created at CNMS. This expertise and our capabilities enable seamless integration of synthesis, characterization, modeling, and data analytics, empowering collaborative discovery and dramatically increasing scientific productivity. Pursuit of our first four goals establishes this foundation and drives leadership in key scientific domains where CNMS's distinctive expertise, instrument innovation, and multidisciplinary workflows align with national priorities.

Fully realizing the promise of autonomous workflows, advanced materials, quantum information science, and AI also requires CNMS to grow and integrate within a broader user facility ecosystem. We will build partnerships that allow coordination, curation, and standardization of datasets; establishment of interoperable workflows; and leveraging of multimodal datasets across SUF Division facilities, academia, and the private sector to create new understanding that ensures the impact of unique CNMS-developed tools and methods scales nationally. Long-term success further depends on combining scientific and technical innovation with operational excellence centered on fostering an engaged user community and an empowered staff equipped to lead this next era of discovery.

Goals	
1	 Transform the practice of collaborative nanoscience through autonomous and data-driven discovery using one-of-a-kind, human-centered experimental platforms
2	 Lead in understanding and utilizing heterogeneities in quantum materials to realize new functional quantum architectures
3	 Harness complex macromolecular conformations to achieve predictive control of polymer function and shape the behavior of soft matter
4	 Decode and direct multiscale dynamics and material transformations revealing new pathways for next-generation microelectronics and other critical technologies
5	 Grow and strengthen integration of the CNMS into the National User Facility Ecosystem
6	 Foster a thriving and forward-looking user community supported by a staff-centric development culture

Goal 1



TRANSFORM THE PRACTICE OF COLLABORATIVE NANOSCIENCE THROUGH AUTONOMOUS AND DATA-DRIVEN DISCOVERY USING ONE-OF-A-KIND, HUMAN-CENTERED EXPERIMENTAL PLATFORMS

Strategic Intent: Establish CNMS as the national leader in collaborative human-AI workflows for materials discovery. Built with the aim of tightening the feedback loop in synthesis, characterization, integration, and modeling, autonomous experimentation is the ultimate expression of this goal. Our vision for this revolution in research does not diminish the role of scientists. Rather, it augments and empowers the scientist and user to explore, discover, and achieve new developments with greater speed and deeper insights that could not be realized otherwise. It is also an integral step in accelerating the creation of reliable and secure multimodal datasets that will fuel the DOE Genesis Mission.

Impact: Integrating synthesis, characterization, modeling, and data analytics within seamless, closed-loop frameworks will dramatically accelerate the pace of discovery, reduce experimental bottlenecks, enable breakthroughs that cannot be accessed through traditional methods, and shorten the path from fundamental insight to impactful applications for CNMS and its users. These systems will augment human intuition with adaptive automation and AI-driven decision-making to explore broader design spaces, uncover hidden correlations, and reveal emergent behaviors with unprecedented speed and precision. This transformation will position CNMS as a national hub for the next generation of intelligent, data-centric research, empowering staff and users to achieve breakthroughs that fundamentally change how materials are understood and engineered.

Why CNMS? CNMS is uniquely positioned to lead this transformation because it has already built a foundation of scientific expertise, infrastructure, and organizational culture required for autonomous, human-centered experimentation. The center has invested deeply in staff capabilities at the intersection of synthesis, characterization, computation, and data science, most notably through the creation of the DNA Group and a unique and growing GPU powered cloud. The foundations of this group in scanning probe microscopy, electron microscopy, and thin-film synthesis provide unparalleled domain expertise for developing AI-driven experimental workflows. These strengths are amplified by tight integration across all CNMS research groups and scientific themes, enabling multidisciplinary problem solving and rapid deployment of autonomous methods across diverse materials systems. Coupled with state-of-the-art instrumentation, user-focused operations, and strategic partnerships with SNS, HFIR, and Oak Ridge Leadership Computing Facility (OLCF), CNMS brings together everything required to pioneer first-of-a-kind platforms and workflows that will define the future of collaborative nanoscience.

Strategic Objectives:

1.1. Develop and deploy closed-loop theory and experimental workflows

- 1.1.1. Pilot autonomous platforms across all three theme research efforts that leverage unique CNMS capabilities across the ORNL campus
- 1.1.2. Establish standards for interoperability between experimental instruments, data systems, and modeling frameworks across the center consistent with FAIR (Findable, Accessible, Interoperable, Reusable) data principles and PuRe (Publicly Reusable Research) resources
- 1.1.3. Achieve measurable improvements in nanoscale synthesis—including increased throughput, enhanced precision, reproducibility, and control of material structure—through AI-assisted design, optimization, and feedback-guided synthesis workflows

1.2. Expand data-driven and AI-assisted research across the user program

- 1.2.1. Increase the proportion of CNMS user and staff projects employing data-driven or AI-assisted methods to $\geq 50\%$ by FY2030
- 1.2.2. Develop and maintain a suite of user-accessible AI tools and model libraries tailored to materials design, image, and spectral analysis as well as experimental optimization
- 1.2.3. Partner with other DOE user facilities and computational centers to co-develop shared Digital Research Environments (DREs) and federated learning frameworks
- 1.2.4. Create targeted training modules and workshops to help users integrate machine learning and automation into their experimental workflows

1.3. Build shared AI/ML infrastructure for materials discovery

- 1.3.1. Establish a timeline for continuous assessment and “right-sizing” centralized compute and storage infrastructure to support distributed AI/ML workflows across CNMS
- 1.3.2. Implement secure cloud-based environments for model training, inference, and workflow orchestration that can be readily accessed by remote and onsite staff and users
- 1.3.3. Launch collaborative projects that co-develop models capable of autonomously predicting materials behavior or optimizing synthesis parameters
- 1.3.4. Implement policies and procedures for systematic capture, curation, and management of experimental data, metadata, and sample provenance

Goal 2



LEAD IN UNDERSTANDING AND UTILIZING HETEROGENEITIES IN QUANTUM MATERIALS TO REALIZE NEW FUNCTIONAL QUANTUM ARCHITECTURES

Strategic Intent: The ability to understand and control *heterogeneities in quantum materials* sits at the intersection of quantum phenomena, defect and interface science, and advanced characterization/modeling, all areas where CNMS is positioned to lead. CNMS will drive fundamental research to reveal and control the heterogeneities, defects, interfaces, dopants, and local structural variations that define and enable functional quantum phenomena. These nanoscale features, while often viewed as imperfections, are essential to the emergent behavior that underpins quantum information systems, quantum sensing, and correlated electronic materials. By combining precision synthesis, multimodal characterization, and predictive modeling, CNMS will elucidate the origins and impact of heterogeneity and transform it into a design principle for next-generation quantum information systems, sensors, and correlated materials.

Impact: By establishing new methods to map, model, and engineer these heterogeneities with atomic-level precision, CNMS will redefine how functional quantum architectures are conceived and realized. Mastering this level of control will enable breakthroughs in coherence, transduction, and emergent quantum behavior, opening pathways to qubits and quantum sensors with unprecedented stability and performance. CNMS will transform heterogeneity from a liability into a powerful design tool, accelerating the understanding and development of quantum technologies that meet national needs in computation, communication, and sensing. This goal responds to growing user demand for integrated capabilities to probe and understand quantum materials and devices across atomic to mesoscale dimensions. By providing coordinated access to synthesis, advanced microscopy, and modeling within unified workflows, this will enable users to uncover the fundamental mechanisms that govern quantum behavior in real materials and devices.

Why CNMS? CNMS is uniquely positioned to lead in this area through its deep expertise in atomic-scale imaging and characterization, including world-recognized strengths in scanning tunneling microscopy, advanced scanning probe methods, and electron microscopy and spectroscopy. These tools are essential for resolving the defects, interfaces, and structural variations governing quantum behavior. These capabilities are tightly integrated with precision quantum-materials synthesis, including directed atomic manipulation using AI-driven scanning tunneling microscopes and scalable growth of transition metal dichalcogenides and other 2D materials that form the foundation for multilayer heterostructures and moiré materials. These experimental strengths are complemented by the Nanomaterials Theory Institute (NTI) Group's advanced multiscale modeling capabilities that connect atomic-level heterogeneities to mesoscopic behavior and device-relevant quantum function. Coupled with access to neutron scattering (SNS/HFIR) and high-performance modeling (OLCF), CNMS provides a unique environment where synthesis, characterization, and predictive theory advance cohesively, enabling controlled exploration and exploitation of heterogeneity in functional quantum materials.

Strategic Objectives:

2.1. Expand workflows for atomically precise characterization, creation, and control of quantum-relevant heterogeneities

- 2.1.1. Continue to advance and integrate complementary probes (e.g., scanning probe microscopy, nitrogen-vacancy center microscopy, scanning transmission electron microscopy, and electron energy loss spectroscopy) to quantify and manipulate local electronic, spin, and structural degrees of freedom
- 2.1.2. Establish coordinated experimental–computational workflows to connect and create observed heterogeneities to emergent behavior and enable their controlled creation across length scales
- 2.1.3. Create and maintain open-access data repositories for defect and interface characterization to accelerate user-driven AI/ML discovery
- 2.1.4. Collaborate with the quantum information science community and industry stakeholders to translate fundamental insights into material platforms for quantum computing, networking, and sensing applications

2.2. Link local structure to emergent quantum functionality

- 2.2.1. Identify and quantify correlations between nanoscale structural variations and macroscopic quantum phenomena such as coherence, entanglement, and charge/spin transport
- 2.2.2. Develop advanced theoretical and simulation frameworks to describe quantum-defect interactions in complex materials environments
- 2.2.3. Support user and staff projects that co-design synthesis, measurement, and modeling to control specific defect-property relationships

2.3. Build a community for quantum heterogeneity science

- 2.3.1. Host cross-facility workshops linking CNMS capabilities with neutron, photon, and computational user facilities
- 2.3.2. Launch a renewed CNMS Quantum Defects and Interfaces Initiative to engage new users and catalyze collaborations through coordinated seminar series, topical workshops, and shared experimental–theoretical workflows.

Goal 3



HARNESS COMPLEX MACROMOLECULAR CONFORMATIONS TO ACHIEVE PREDICTIVE CONTROL OF POLYMER FUNCTION AND SHAPE BEHAVIOR OF SOFT MATTER

Strategic Intent: CNMS will lead the discovery and design of polymeric materials in which non-equilibrium conformations, arising from electrostatics, topology, and processing, are *predictably linked* to macroscopic performance. The HCMC theme aims to unify precision, automated synthesis, in situ characterization, and predictive modeling to transcend traditional tradeoffs between performance and control. By establishing physics-based design rules for complex macromolecular systems, CNMS will enable next-generation polymer materials that combine high performance, cost effective, and tunable responsiveness to stimuli such as flow and electric fields.

Impact: By revealing how electrostatics, topology, and processing history shape non-equilibrium chain behavior and by turning those relationships into actionable design rules, CNMS will enable the creation of polymer systems that break longstanding performance tradeoffs, deliver faster and more efficient responses, and adapt their function across soft-hard interfaces. This capability will open new pathways for high-performance materials for energy storage and transduction, flexible electronics, and next-generation structural and functional composites. This goal will strengthen user access to integrated synthesis, deuteration, multimodal characterization, and modeling capabilities needed to understand and control soft and hybrid materials across scales. By embedding AI/ML-enabled workflows and expanding the scope of accessible tools, work will empower users to investigate complex macromolecular behavior and advance fundamental understanding through collaborative, data-rich research.

Why CNMS? CNMS offers an exceptional combination of precision polymer synthesis, deuteration, modeling and interpretation of advanced neutron-enabled soft-matter characterization, and nanoscale imaging. The center's strengths in ionic, zwitterionic, and topologically complex polymer and copolymer synthesis, together with AI-driven flow synthesis capabilities in the Macromolecular Nanomaterials Group, provide a unique foundation for systematically tuning conformations and interactions. These capabilities are deeply integrated with multimodal characterization, including neutron scattering at SNS and HFIR, high-speed and multimodal scanning probe microscopy, and in situ quartz crystal microbalance (QCM)-based and optical platforms that capture polymer dynamics across wide temporal and spatial ranges. Complementary multiscale modeling from the Nanomaterials Theory Institute and use of neutrons for probing structure and dynamics at the nanoscale enables direct connection between molecular structure and macroscopic response. This cohesive environment allows CNMS to iteratively synthesize, measure, and model complex macromolecular systems, positioning the center to lead nationally in predictive soft-matter design and control.

Strategic Objectives:

3.1. Expand predictive frameworks for understanding non-equilibrium chain conformations of polymers in changing environments

- 3.1.1. Expand and refine synthesis capabilities to broaden the variety of deuterated materials and polymers with precisely controlled structures and reduce their development timelines
- 3.1.2. Employ neutron and X-ray scattering for probing structure and dynamics, multi-modal imaging and spectroscopy, and molecular simulation to capture structure-function relationships across multiple length and time scales in soft-matter systems
- 3.1.3. Create and benchmark predictive, physics-informed models capable of forecasting chain conformations and response under non-equilibrium conditions
- 3.1.4. Identify and quantify the molecular mechanisms by which topology and charge mediate energy dissipation and relaxation in polymers under driving fields

3.2. Leverage machine-learning and data-driven modeling to advance polymer synthesis and characterization

- 3.2.1. Apply machine-learning and data-driven modeling to uncover hidden correlations between kinetics of polymerization, copolymerization, emergent structure, and dynamics for polymer solutions of interest to the user community including deuterated polymers
- 3.2.2. Validate predictive design principles through iterative synthesis-characterization-modeling feedback loops
- 3.2.3. Study the effects of deuteration on properties of polymer solutions and melts

3.3. Advance cross-facility and multi-modal integration

- 3.3.1. Leverage CNMS's partnerships with neutron facilities (HFIR, SNS) to probe polymer dynamics, topology, and electrostatics in situ
- 3.3.2. Integrate neutron scattering data with computational models and CNMS-based characterization to create holistic, cross-scale descriptions of polymer behavior
- 3.3.3. Establish collaborative projects across DOE NSRCs to align polymer and soft-matter research efforts and share predictive modeling infrastructure
- 3.3.4. Position CNMS as a nexus for predictive polymer science within the DOE user facility network by elevating theory and computation as core user-facing capabilities, developing integrated experiment-modeling workflows, and supporting these efforts through targeted outreach, shared modeling resources, and focused user workshops on non-equilibrium soft matter.

Goal 4



DECODE AND DIRECT MULTISCALE DYNAMICS AND MATERIAL TRANSFORMATIONS REVEALING NEW PATHWAYS FOR NEXT-GENERATION MICROELECTRONICS AND OTHER CRITICAL TECHNOLOGIES

Strategic Intent: CNMS will advance the understanding and control of how energy, in electronic, vibrational, and magnetic states, flows within and across materials and interfaces. It will, in turn, predict and understand associated material transformations that accompany these processes. These processes govern functionality in next-generation microelectronics and quantum devices but are also inherent in the integration and fabrication protocols required for their realization. By integrating new experimental capabilities, predictive modeling, and cross-facility collaboration, CNMS will build a foundation for designing and controlling energy transport from atoms to applications and harness these findings to work with stakeholders to achieve new levels of functionality.

Impact: Working at the nanoscale enables access to extreme energy densities, delivered through focused beams, ultrafast pulses, and scanning probe tips, that can drive rapid transformations, generate metastable states, and unlock functionalities inaccessible at equilibrium. By decoding how electronic, vibrational, magnetic, and structural energy flows and dissipates across materials and interfaces, CNMS will identify new ways to direct these transient states toward enhanced performance. Understanding how materials evolve during operation and throughout complex fabrication processes will inform new device architectures and processing strategies. Through integrated in situ diagnostics, autonomous synthesis, and AI-driven characterization platforms, CNMS will establish predictive control over dynamic behavior from the atomic to the device scale, enabling the discovery of materials and heterostructures that deliver fundamentally new modes of functionality for next-generation microelectronics and quantum technologies. Aligned directly with the Multiscale Dynamics research theme, achieving this goal will provide users with integrated, time-resolved and multimodal capabilities to study material transformations under realistic conditions, enabling fundamental insight into dynamic behavior across thin films, interfaces, and nanostructured systems.

Why CNMS? The center combines precision and autonomous synthesis with advanced characterization tools capable of delivering and measuring high energy densities in controlled ways, from ultrafast laser pulses and electron beams to scanning probe tips that can write, erase, and manipulate functionalities such as ferroelectric domains. These tools are deeply integrated with cryogenic and operando imaging, fast multimodal probes, and emerging time-resolved neutron-based techniques at SNS and HFIR. This enables CNMS to capture the formation, evolution, and relaxation of metastable states that govern device behavior. AI/ML-driven data pipelines and multiscale modeling from NTI connect local transformations to long-range dynamics and device-relevant properties. Together, this uniquely cohesive environment, spanning synthesis, manipulation, detection, and theory, positions CNMS to reveal and control the dynamic processes that underpin next-generation microelectronics and quantum devices.

Strategic Objectives:

4.1. Develop and integrate advanced capabilities for probing dynamic energy transport across scales

- 4.1.1. Establish multimodal platforms that couple ultrafast optical, scanning probe, and neutron-based techniques to capture charge, spin, and phonon dynamics from femtoseconds to seconds and nanometers to microns
- 4.1.2. Build correlative data and modeling workflows to connect local excitations and energy flow during material etching/manipulation, integration, and device operation with device-relevant structures and interfaces

4.2. Uncover fundamental mechanisms governing coupled electronic, phononic, and magnetic dynamics

- 4.2.1. Use precision synthesis, *operando* measurement, and predictive modeling to elucidate how atomic structure, defects, strain, and interfaces govern the transfer, conversion, and dissipation of energy
- 4.2.2. Develop physics-based models to predict and control coherence, transport, and relaxation processes that underpin functionality in quantum and microelectronic materials

4.3. Enable cross-facility integration and a user-centered multiscale dynamics program

- 4.3.1. Leverage CNMS partnerships with HFIR, SNS, and other DOE user facilities to create coordinated measurement and data platforms that span time and length scales
- 4.3.2. Engage users through focused outreach, workshops, and joint experiments to expand community access to multimodal dynamic measurements and modeling infrastructure

Goal 5



GROW AND STRENGTHEN INTEGRATION OF THE CNMS INTO THE NATIONAL USER FACILITY ECOSYSTEM

Strategic Intent: CNMS will strengthen its role as a gateway for multi-facility, multi-modal discovery while also defining a clear and distinct role for the center within the SUF Division ecosystem of light and neutron sources and NSRCs. The CNMS will clearly define signature capabilities aligned with scientific theme research and group capabilities that complement the other NSRCs, while expanding partnerships and coordinating efforts across the network.

Impact: Strengthening CNMS's coordination across the national user facility ecosystem will amplify the impact of both CNMS science and the broader DOE research enterprise while providing CNMS and its partners to standardize best practices for data collection and management. By building coordinated, multi-modal workflows across SUF Division facilities and defining CNMS's signature capabilities, these efforts will help establish seamless pathways for discovery that span synthesis, characterization, and theory. Deeper integration will not only accelerate materials discovery through interoperable data, cross-facility learning, and the Genesis platform vision but also enable CNMS users and staff to benefit from expanded access to complementary capabilities and collaborative research teams. Through more coordinated engagement with the NSRC network, light sources, neutron facilities, and computational centers, CNMS will broaden its scientific reach, enhance the collective strength of the national user facility ecosystem, and facilitate access for users across the network.

Why CNMS? CNMS is well positioned to be a major contributor to an integrated national user facility ecosystem due to its distinctive combination of domain expertise, signature capabilities, and strategic location within ORNL. The center offers unique strengths in multimodal characterization, advanced polymer and quantum materials synthesis, autonomous and data-driven experimentation, and deuteration-enabled soft-matter research. These signature capabilities include, for example, atomic-scale imaging, spectroscopy, and manipulation across multiple modalities; strong integration of soft-matter and quantum materials science with neutron scattering; development of unique, agent-operated autonomous experimental setups incorporating theory-in-the-loop; and a GPU-powered data cloud that enables end-to-end materials discovery. [see Appendix B for signature capabilities listed by group]. These strengths generate high-value datasets that complement and extend capabilities across the NSRCs, neutron sources, and light sources. CNMS's proximity to SNS, HFIR, and OLCF facilitates natural cross-facility workflows, while its established user program provides a strong foundation for collaborative projects that bridge institutions. Increased integration will, in turn, benefit CNMS by expanding access to complementary tools, enabling shared data standards, and strengthening partnerships that enhance user support, scientific breadth, and national impact.

Strategic Objectives:

5.1. Coordinate alignment to enhance cross-facility collaborations with SNS/HFIR

- 5.1.1. Roadmap, establish, and expand deuteration and isotopic substitution capabilities
- 5.1.2. Develop coordinated workflows to guide staff and users toward integrated sets of complimentary modeling, characterization, and synthesis capabilities at CNMS and SNS/HFIR to increase cross-facility use and collaboration
- 5.1.3. Establish a central theory and AI/ML hub as a unifying platform for supporting data-driven analysis and simulation across NSRCs and neutron facilities
- 5.1.4. Launch annual collaborative cross-facility user projects (three per year) to demonstrate integrated workflows

5.2. Build interoperable cross-facility data frameworks and mechanisms for collaboration and networking

- 5.2.1. Coordinate, develop, and implement SUF Division-wide data standards, user agreements, and FAIR data repositories
- 5.2.2. Support development of a universal NSRC proposal process that formalizes and coordinates multi-center access, including a common submission or data-sharing portal that allows proposals from one facility to be efficiently translated to sister facilities
- 5.2.3. Host semi-annual “capability workshops” to align facility investments, share technical best practices, and identify opportunities for co-development with NSRCs

5.3. Expand outreach, education, and engagement across the user facility ecosystem

- 5.3.1. Develop cross-facility outreach, education, and joint training initiatives to broaden recognition of NSRC capabilities and partnerships across the scientific community.
- 5.3.2. Expand partnerships with industry to accelerate technology translation
- 5.3.3. Modernize and redesign the CNMS web presence to more effectively showcase facility capabilities, staff expertise, and user pathways, leveraging the upcoming web migration to improve visibility, accessibility, and engagement with academic, industry, and government research communities.

Goal 6



FOSTER A THRIVING AND FORWARD-LOOKING USER COMMUNITY SUPPORTED BY A STAFF-CENTRIC DEVELOPMENT CULTURE

Strategic Intent: CNMS will cultivate a vibrant and collaborative user community by investing in the growth and engagement of its staff. Recognizing that exceptional user experiences stem from empowered, well-trained personnel, CNMS will establish a culture of continuous learning, effective communication, and empower staff with the tools, training, and support needed to engage more effectively as collaborative scientific partners to our users. Through targeted development programs, enhanced outreach, and data-informed evaluation, CNMS will strengthen the connection between staff expertise and user success, ensuring that every user interaction reflects the center's commitment to scientific impact, teamwork, and integrity. CNMS will ensure that staff and users alike are engaged and prepared to embrace data-driven, autonomous materials research and to collaborate effectively across scientific disciplines and institutions.

Impact: Empowering staff is fundamental to the success of CNMS and to the quality and impact of its user program. By investing in professional development, mentoring, and opportunities for staff to broaden their scientific and collaborative skills, CNMS will ensure that its workforce is well prepared to engage users across diverse disciplines and evolving research needs. Modern data systems and digital tools, including automation and AI where appropriate, will be deployed to reduce administrative burden, improve coordination, and support more effective communication, allowing staff to focus on scientific engagement and problem solving. Together, these efforts will strengthen the user experience, enhance staff effectiveness and satisfaction, and cultivate a culture in which CNMS personnel are empowered to lead, innovate, and grow alongside the scientific community they serve.

Why CNMS? CNMS has a long-standing strength in working closely with users to design, execute, and interpret complex experiments, and this goal builds directly on that foundation. A thriving user community depends on a staff that is well supported, well trained, and empowered to collaborate across disciplines and facilities. CNMS has already demonstrated leadership in building teams that can operate in AI-enabled research spaces, from autonomous synthesis and advanced microscopy to multimodal data integration. Extending this mindset to staff development and user engagement will allow CNMS to harness emerging AI/ML tools to streamline user interactions, enhance project coordination, improve outreach, and strengthen the overall effectiveness of the user program. By investing in its people, CNMS not only improves its operational excellence but also builds the workforce and culture necessary to lead in the next era of autonomous and data-centric scientific discovery.

Strategic Objectives:

6.1. Equip and train staff and users to conduct highly multidisciplinary research that leverages emerging AI/ML, data-driven workflows and in-house built, custom-instrumentation

- 6.1.1. Develop user training and staff upskilling programs on AI-driven materials research and automation
- 6.1.2. Develop a structured program to support and reward in-house design, fabrication, and deployment of custom detectors and research instrumentation as a core capability enabling differentiated user and theme science.
- 6.1.3. Enhance staff onboarding, professional development, and training to augment scientific expertise with top-tier outreach and customer service based on the principle that everyone is an ambassador
- 6.1.4. Establish a structured *Staff Development and Training Program* focused on user engagement, communication, and leadership
- 6.1.5. Equip staff with outreach media and materials that complement our scientific and user facility mission while increasing CNMS visibility through coordinated communications (web presence, user stories, joint seminars) with a goal of 25% growth in digital engagement metrics by FY2028

6.2. Establish a culture of feedback that solicits and uses input from stakeholders to guide best practices in execution of user projects and outreach

- 6.2.1. Incorporate user feedback metrics (e.g., satisfaction scores, collaboration indices) into staff performance and recognition frameworks
- 6.2.2. Develop and implement a CNMS “User Engagement Framework” to standardize onboarding, communication, and post-project interactions with users
- 6.2.3. Establish a CNMS “User Ambassador” program by FY2027 to connect staff and experienced users with emerging research communities

6.3. Demonstrate continued operational excellence and stewardship of resources that optimize impact with uncompromised safety

- 6.3.1. Establish metrics and goals for safety, instrument uptime, user productivity, and resource utilization, and review them quarterly to drive evidence-based decisions and optimize facility operations.
- 6.3.2. Develop a structured process for assessing equipment health, prioritizing upgrades, and aligning capital investments with long-term scientific impact, ensuring reliable operations and sustained leadership in nanoscience capabilities.

Implementation and Investment Plan

This Implementation and Investment Plan translates our strategic vision into actionable steps, guided by clear principles that ensure alignment, accountability, and impact. The implementation of this strategic plan is structured around four interconnected efforts that translate CNMS's vision into coordinated action: (1) a center-wide initiative to drive autonomous experimentation and AI-integrated research workflows; (2) the scientific themes that drive multidisciplinary discovery and map directly onto Goals 2–4; (3) enhanced outreach and ecosystem integration that strengthen CNMS's role within the SUF Division network; and (4) staff-centric development programs that enable effective user engagement and operational excellence. Together, these subsections outline how the center will build the capabilities, infrastructure, partnerships, and workforce required to support autonomous, data-rich discovery while advancing frontier science across quantum materials, polymers, and multiscale dynamics. They also establish the foundation for generating, curating, and sharing high-value multimodal datasets, expanding national partnerships, and cultivating a thriving staff and user community, all essential for achieving the goals outlined in this plan. Our investment strategy outlines priority investments and activities for each goal and identifies key risks and mitigation strategies to support successful execution.

This implementation and investment plan is intentionally ambitious yet grounded in a clear understanding of current and future resource constraints. It was developed with full recognition that budgets, schedules, and national priorities may evolve over time, and is therefore structured to remain flexible and adaptive under a range of funding scenarios. The strategic goals and associated investments are achievable within a stable funding environment, while the prioritization framework established through this planning process provides guidance for scaling, sequencing, or adjusting activities as needed. By emphasizing modular investments, dual-use capabilities, and cross-cutting infrastructure that benefits multiple goals, CNMS will remain agile, able to respond to changing conditions while continuing to deliver high-impact science and user value in support of DOE mission priorities.

Cross-Cutting Initiative: Advancing Autonomous Experimentation and AI-Integrated Nanoscience



Advancing Goal 1. CNMS has long served as a national steward for cutting-edge synthesis, characterization, and modeling. The next stage of this leadership requires deeply embedding autonomous experimentation and AI/ML-driven analysis into the fabric of how science is conducted. This cross-cutting initiative reflects our commitment to developing one-of-a-kind experimental platforms and adapting commercial systems to support a new paradigm in human-centered, data-driven discovery. These capabilities are not isolated tools but foundational elements that amplify all CNMS science, enabling researchers to explore broader experimental spaces, capture transient phenomena, and accelerate insight through real-time decision-making.

Implementing this vision demands a coherent digital and operational framework across the center. CNMS will therefore prioritize standardizing workflows, data movement, storage, and analysis to ensure that autonomous systems can interact seamlessly with each other and with human researchers. Establishing this shared infrastructure will allow the center to generate high-quality, richly annotated multimodal datasets that are essential for training AI models, validating digital twins, and enabling rapid materials discovery. Moreover, these rich, diverse multimodal datasets are critical for AI-driven hypothesis generation, providing the context needed to reveal mechanisms and structure–property relationships. These efforts support and operationalize Goal 1 while strengthening the scientific themes that follow, ensuring that CNMS remains at the forefront of next-generation research methodologies that seamlessly connect synthesis, characterization, modeling, and human expertise in a unified autonomous discovery ecosystem.

To embed autonomy and AI/ML across the center, CNMS will prioritize hiring staff with expertise in AI-enabled research and autonomous experimentation while creating opportunities to upskill staff and users in the same competencies. We will invest in instruments and control systems designed for real-time data capture, seamless integration into autonomous workflows, and rigorous sample provenance tracking. CNMS will continue to expand and refine its unique user-accessible cloud environment with GPU resources, enabling scalable AI/ML model training and near-real-time analysis. These investments will be deployed broadly across the scientific themes, the user program, and even facility operations, ensuring that AI-driven methods enhance experimental design, support cross-facility workflows, and strengthen staff development and outreach. In doing so, CNMS will establish unified and forward-looking research infrastructure that amplifies all subsequent goals while positioning the center as a leader in the integration of autonomy and AI within the national user facility ecosystem.

Theme Science: Coordinating Expertise for Multidisciplinary Discovery

Advancing Goals 2-4. CNMS is organized to foster collaboration across disciplinary boundaries, connecting fundamental understanding with advanced synthesis, fabrication, and characterization. Eight groups collectively provide an end-to-end host of capabilities, facilities, and depth of scientific expertise. This structure ensures efficient coordination of resources, effective mentoring and development of staff, and rigorous evaluation and support of user projects. By maintaining deep technical expertise and operational stability, the groups provide the foundation of excellence from which the scientific themes draw their rigor, integration, and innovation. A full accounting of the broad capabilities stewarded by the groups can be found on the CNMS website at <https://www.ornl.gov/facility/cnms>. Summaries provided in Appendix B highlight each group's core expertise, unique capabilities, and alignment with CNMS strategic goals. The groups serve as the primary interface for users, while also providing the foundation for staff development and a seamless, high-quality user experience (Goal 6).

Their work is coordinated across three cross-cutting and evolving **scientific themes** that define CNMS's research identity, align with our strategic goals, and support our user program:



Heterogeneities in Quantum Materials (HQM): Understanding how local structural alterations and electronic variations impact collective and emergent quantum behavior



Harnessing Complex Macromolecular Conformations (HCMC): Designing and controlling hierarchical architectures in soft and hybrid matter to realize novel functions



Multiscale Dynamics (MD): Revealing the links between energy transport and the temporal and spatial evolution of functional materials across atomic to macroscopic scales

Together, this structure ensures both deep technical excellence and flexible scientific integration. It enables CNMS to respond nimbly to emerging opportunities and shifting national priorities while sustaining the mission of providing world-class user access to advanced nanoscience capabilities. Development of signature capabilities within the groups and complex multidisciplinary workflows across the themes provides the basis for defining a unique role for the CNMS within the user facility ecosystem. The three CNMS scientific themes map directly onto Goals 2–4, providing the foundational scientific drivers for research in quantum materials, complex macromolecular systems, and multiscale dynamics while also informing and strengthening the broader center-wide goals in autonomy, ecosystem integration, and user community development.

CNMS operates under a dual scientific mission to deliver world-leading capabilities for the user community while advancing foundational research that drives the future of nanoscience. Within this mission, the scientific themes serve as the framework for fostering and refining multidisciplinary work and workflows across the center. They create a proving ground where

capabilities originating within individual groups are integrated to achieve deeper, system-level understanding of materials and phenomena. The themes are intentionally aligned with national priorities and DOE BES research directions, addressing critical knowledge gaps that currently limit the translation of materials discoveries into practical solutions.

The themes are tightly intertwined with the user program. They act as testbeds for developing and demonstrating new cross-disciplinary workflows that can be transitioned into user-accessible capabilities, ensuring CNMS science evolves with user needs. For staff scientists, the themes provide an opportunity to expand their expertise, cultivate agility in working across disciplines, and gain a broader perspective on how their science connects to that of others, enhancing both individual and institutional impact.

Themes are selected and evolved to align with emerging national needs, harness unique strengths within CNMS, and catalyze the development of new tools and methods valued by users and staff. They represent areas where a critical mass of expertise, infrastructure, and momentum already exists, within both internal staff and the user community, such that strategic investment can quickly accelerate progress and amplify impact. Importantly, the themes are dynamic by design, evolving through regular center-wide discussions and town halls that encourage idea exchange, coordination, and the identification of new opportunities. The themes are also reviewed and adjusted in consultation with our scientific advisory committee. This adaptive approach ensures that CNMS remains responsive to the evolving frontiers of nanoscience and continues to lead in building the multidisciplinary foundations for materials discovery.

A brief description of each theme, its relevance to national and BES priorities, and its alignment with our strategic plan is provided below.



UNDERSTAND & UTILIZE HETEROGENEITIES IN QUANTUM MATERIALS

Goal 2: Understanding, controlling, and exploiting nanoscale defects, interfaces, and disorder to create, preserve, and manipulate emergent quantum phenomena

Overarching goal and vision: The HQM theme seeks to uncover how structural imperfections, interfaces, and nanoscale heterogeneities give rise to emergent quantum states and how these features can be deliberately tailored to achieve collective and functional control. The overarching goal is to understand the formation, behavior, and coherence of quantum states in low-dimensional and heterogeneous systems through nanoscale manipulation of defects, interfaces, and disorder. By combining atomic-scale measurement, deterministic modification, and predictive theory, HQM aims to reveal and engineer the interplay of structure, symmetry breaking, and quantum correlations that underpin quantum materials and devices for computation, sensing, and communication.

HQM integrates the expertise of CNMS groups in scanning probe and electron microscopies (the Scanning Tunneling Microscopy [STM], Functional Atomic Force Microscopy [F-AFM], and electron Microscopy and MicroAnalysis [eMMA] Groups), synthesis (the Functional Hybrid Nanomaterials [FHN] and Nanofabrication Research Laboratory [NRL] Groups), and theory (the NTI group) to achieve atomic-scale characterization, precision synthesis, and multiscale modeling of quantum phenomena. This integration places CNMS at the forefront of understanding how quantum states emerge and evolve in complex material systems ranging from van der Waals heterostructures and correlated magnets to molecular and defect-engineered platforms.

Relevance to national and BES priorities: The HQM theme directly supports DOE and BES priorities in quantum materials for energy-relevant technology, next-generation quantum systems, and microelectronics. The ability to control and utilize quantum coherence, entanglement, and spin phenomena underpins future advances in quantum information science (QIS), sensing, and secure communication. HQM contributes to these national missions by linking fundamental discovery of quantum states to practical strategies for robust, scalable, and functional quantum systems. The theme also complements ongoing DOE initiatives in cross-facility quantum materials research, leveraging CNMS's co-location with SNS, HFIR, and OLCF to enable multimodal exploration of quantum structure and dynamics across length and time scales.

Strategic realignment and integration: HQM is being realigned to enhance scientific cohesion and strengthen integration with both user-driven research and DOE's quantum priorities. The realignment elevates HQM into a coherent, goal-oriented framework focused on the quantum roles of heterogeneities as a deliberate design principle. Rather than treating disorder as a limitation, HQM embraces controlled heterogeneity as a transformative opportunity to stabilize, manipulate, and coherently transduce information carriers for networking, sensing, and computing architectures.

The realigned theme encompasses moiré materials, low-dimensional heterostructures, atomically ordered model systems that enter regimes dominated by the quantum behavior of defects, boundaries, and interfaces. A key emphasis is placed on connecting structural and electronic heterogeneity to coherence and decoherence pathways, essential for advancing quantum information and sensing technologies. HQM prioritizes material platforms that present clear routes to functional devices. HQM will expand efforts in correlative microscopy and spectroscopy, combining STM, AFM, and electron microscopy with ultrafast and low-frequency optical probes to link atomic-scale structure with dynamic quantum responses. These experiments will be guided by first-principles and ML-enabled simulations, providing a predictive framework for designing quantum materials where heterogeneity is a controllable and optimizable feature.

This refinement also strengthens HQM's integration with the user program and neutron facilities. By connecting CNMS's nanoscale characterization and synthesis tools to neutron and X-ray studies of spin, lattice, and electronic excitations, HQM will support multi-modal exploration of quantum phenomena spanning local to collective scales. This strategy enhances cross-facility partnerships by providing users with cohesive pathways from atomic insight to device-relevant measurements.

Impact on User Program: HQM directly addresses growing user demand for atomic- to mesoscale characterization of quantum materials, particularly those involving engineered defects, interfaces, and low-dimensional architectures. Users increasingly require integrated access to synthesis, microscopy, and modeling tools that can quantify and manipulate quantum coherence and spin phenomena in real materials. By building workflows that combine STM, AFM, and electron microscopy with theoretical modeling and data-driven analysis, HQM provides users with a pathway from discovery to design. The theme also supports DOE's growing community of QIS users by providing experimental testbeds and training opportunities that link quantum materials synthesis, characterization, and modeling within a collaborative, user-driven framework.

Connections to CNMS strategic goals: In addition to being squarely aligned with Goal 2, efforts in the theme integrate across the center's strategic goals in the following ways:

Goal 1 – HQM leverages AI/ML-driven control and analysis to automate quantum material exploration—linking data from microscopy, spectroscopy, and modeling to accelerate discovery of heterogeneity-induced phenomena.

Goal 5 – HQM strengthens integration with SNS, HFIR, and OLCF by bridging atomic-scale characterization with neutron and computational studies of collective excitations, coherence dynamics, and emergent order, reinforcing CNMS's cross-facility leadership in quantum materials.

Goal 6 – HQM fosters a growing community of quantum materials users through workshops, tutorials, and joint projects focused on correlative, multimodal characterization. The theme also empowers staff to pursue “quantum materials by design”, using heterogeneity as a new design tool that bridges synthesis, microscopy, and theory boundaries, building expertise in QIS-relevant materials and cultivating the next generation of multidisciplinary researchers.



HARNESS COMPLEX MACROMOLECULAR CONFORMATIONS

Goal 3: Designing, understanding, and controlling the structure and dynamics of macromolecules and hybrid soft materials to enable emergent functionality across scales

Overarching goal and vision: The HCMC theme seeks to link molecular composition of macromolecules to the conformational and assembly dynamics in macromolecular and hybrid materials, exploring how these hierarchical properties give rise to emergent functional properties. This theme integrates macromolecular synthesis, deuteration, characterization, theory, and neutron scattering to reveal the multiscale connections between molecular structure, nanoscale morphology, and macroscopic behavior. Through close coupling of synthesis, in situ characterization, and modeling, HCMC aims to develop predictive control over the structure-

function relationships that determine mechanical, electronic, and transport phenomena in soft and hybrid systems with the broader goal of understanding and mitigating conventional tradeoffs in material function.

HCMC provides the scientific foundation for advancing next-generation soft materials used in energy storage, antifouling sensing, separations, and adaptive technologies. It unites the Macromolecular Nanomaterials (MACRO), FHN, NRL, eMMA, and NTI groups, leveraging CNMS's integrated expertise in polymer design, hybrid interface fabrication, advanced imaging, and multiscale simulation

Relevance to national and BES priorities: This theme directly supports BES's priorities in Basic Research Needs in Synthesis Science for Energy Relevant Technology, Transformative Manufacturing, Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning. The ability to synthesize, understand, and engineer macromolecular structure and dynamics underpins innovations in sustainable polymers, soft electronic interfaces, and hybrid architectures that combine organic and inorganic functionality. The theme contributes to national priorities in materials and AI/ML-enabled synthesis, aligning with DOE goals. The modeling, characterization workflows, and deuteration capabilities developed within this theme directly strengthen the integration between CNMS and SNS/HFIR.

Strategic realignment and integration: The HCMC theme is being realigned to reflect the full breadth of CNMS's capabilities in soft and hybrid materials while sharpening its scientific focus. Rather than concentrating narrowly on a single class of macromolecules (i.e., polyelectrolytes), HCMC will encompass a broader range of charged polymers and architecturally complex systems designed to exhibit tailored responses and controlled assembly in diverse environments. The overarching goal is to minimize conventional tradeoffs in soft, responsive materials by linking molecular topology and composition to emergent mechanical, electronic, and transport behavior. A renewed emphasis will be placed on understanding how these materials behave at, and can be integrated with, hard interfaces, where CNMS's unique ability to characterize and tune surface topography and chemistry provides a distinct advantage. These interfaces are central to hybrid material systems that bridge soft and quantum functionalities. The theme also incorporates a growing focus on deuteration science, both as a cornerstone of neutron-enabled studies and as a driver for expanding CNMS's synthetic and analytical capabilities. By combining AI/ML-guided design with advanced flow chemistry, this effort will accelerate the development of deuterated and isotopically labeled macromolecules, enabling predictive, cross-scale understanding of soft matter and hybrid systems relevant to BES priorities and the broader user community.

Impact on the User Program: This realignment of HCMC strengthens its connection to the CNMS user community by directly addressing growing demand for advanced synthesis, characterization, and modeling of soft and hybrid materials. Users increasingly seek integrated access to deuteration, polymer design, and multimodal characterization capabilities that link nanoscale structure to macroscopic function. By expanding the theme's scope and embedding AI/ML-driven workflows, HCMC will deliver tools and expertise that empower users to tackle complex problems in responsive and hybrid materials. This integration ensures that theme-driven science not only

advances fundamental understanding, but also continuously evolves through user collaboration, feedback, and co-development of new capabilities.

Connections to CNMS strategic goals: In addition to being squarely aligned with Goal 3, efforts across the theme integrate across the center's strategic goals in the following ways:

Goal 1 – HCMC integrates AI/ML with automated synthesis and operando characterization to accelerate discovery of macromolecular design rules and understanding of functionality. Continuous-flow polymerization, coupled with ML-driven feedback, will enable autonomous exploration of compositional and conformational space.

Goal 5 – Through deuteration and soft-matter synthesis, HCMC connects directly to neutron scattering at SNS and HFIR, enabling multimodal investigations of dynamics and structure. Collaborations with OLCF will extend these studies to multiscale modeling and data-intensive analysis, creating a seamless cross-facility workflow.

Goal 6 – HCMC will cultivate a vibrant community of soft- and hybrid-materials researchers through workshops, user calls, and joint neutron-CNMS projects. Internally, the theme provides mentorship and training in polymer synthesis, characterization, and data science for early-career staff and postdocs.



DIRECT MULTISCALE DYNAMICS & TRANSFORMATIONS

Goal 4: Understanding and controlling dynamic processes across length, time, and energy scales to accelerate the design and realization of functional outcomes in energy, quantum, and microelectronics

Overarching goal and vision: The MD theme seeks to build a predictive understanding of how materials evolve during synthesis, processing, operation, and long-term use and to connect these transformations directly to performance. Materials that underpin microelectronics, energy technologies, and emerging functional platforms are shaped by dynamic processes that span vast ranges of time, length, and energy scales. These include ultrafast electronic and vibrational responses, defect migration and reconfiguration, evolving strain fields, and slow chemical or structural aging. The MD vision is to link atomic-scale events to nanoscale morphology and mesoscale function through quantitative frameworks that capture both rapid and gradual mechanisms. By illuminating how materials transform across these scales, MD aims to accelerate the design of next-generation functional materials and enable more efficient and reliable material lifecycles.

This theme unites CNMS strengths in advanced scanning probe techniques, in situ microscopy, spectroscopy, precision synthesis, and multiscale computation to interrogate and control nonequilibrium behavior in materials. Within this integrated framework, MD focuses on defects, strain fields, and interfacial structures as dynamic elements that evolve during growth and respond to external stimuli such as electric fields, mechanical loading, optical excitation, and thermal gradients. Their formation, redistribution, and long-term evolution critically shape the stability and adaptability of functional materials. MD also examines how the structural landscape at two- and three-dimensional interfaces changes under perturbations—such as variations in lattice alignment, symmetry breaking, or processing conditions—and how these evolving environments govern material response. Through coordinated advances in real-time characterization, autonomous experimentation, and multiscale modeling, MD seeks to reveal the mechanisms driving structural and chemical evolution and to establish pathways for intentionally guiding these transformations.

Relevance to National and BES Priorities: The MD theme directly aligns with BES Basic Research Needs in Synthesis Science for Energy-Relevant Technology, Innovation and Discovery of Transformative Experimental Tools, and Microelectronics for Energy-Efficient Computing. These priorities emphasize understanding how materials respond to nonequilibrium environments that arise during growth, integration, and operation. Dynamic processes such as defect redistribution, strain evolution, and interfacial reorganization strongly influence stability and long-term reliability in systems critical to national energy and microelectronics goals. By revealing the mechanisms that govern these transformations, MD supports DOE's vision for innovative materials-by-design, addressing the critical need for predictive understanding of material behavior during processing, and operation.

Strategic realignment and integration: The MD theme is being refined to strengthen coherence and establish a unifying framework for investigating dynamic processes across CNMS's diverse materials platforms. Rather than treating dynamic behavior as an isolated phenomenon, the theme emphasizes a continuous view of material evolution that begins with synthesis and extends through device operation, environmental exposure, and end-of-life processes. This perspective extends the theme's reach to the dynamic processes that govern fabrication, operation, and degradation of functional materials and devices, areas increasingly critical to creating real solutions for microelectronics, quantum information systems, and energy technologies.

Emphasis will be placed on enhancing temporal resolution in microscopy and spectroscopy, expanding computational frameworks for modeling non-equilibrium behavior, and embedding AI/ML approaches to identify, quantify, and predict dynamics. The integration of in situ and operando characterization with autonomous modeling will enable the identification of critical mechanisms that control functionality and failure, providing pathways to accelerate discovery and improve material reliability. Through this realignment, MD becomes a bridge between material synthesis, device fabrication, and operational science, positioning CNMS as a leader in understanding and engineering transformations that define real-world material performance and inviting new partnerships.

Impact on the User Program: The MD theme directly addresses user demand for in situ, time-resolved, and data-rich characterization and modeling of materials under realistic operating conditions. By combining multimodal microscopy, autonomous control, and theory-guided modeling, MD will deliver new workflows that empower users to study transformations relevant to their systems, whether in thin films, hybrid interfaces, or nanostructured devices. These capabilities will enhance CNMS's value to user communities working in microelectronics, energy storage, and catalysis, providing insights into the mechanisms that drive performance and degradation. Theme-driven integration ensures that new tools and methods developed within MD rapidly translate into user-accessible capabilities, expanding opportunities for collaboration and cross-facility research.

Connections to CNMS strategic goals: In addition to being squarely aligned with Goal 4, efforts across the theme integrate across the center's strategic goals in the following ways:

Goal 1 – MD integrates AI/ML and automation with in situ microscopy, spectroscopy, and modeling to identify and predict material transformations in real time, enabling autonomous experimentation and discovery.

Goal 5 – By focusing on material transformations during synthesis and operation, MD connects CNMS directly to neutron and photon user facilities, providing complementary temporal and spatial insights that bridge from atomic dynamics (CNMS) to ensemble behavior (SNS/HFIR). Collaborations with OLCF enhance this integration through large-scale modeling of dynamic processes.

Goal 6 – MD fosters collaboration among users and staff through workshops and training on time-resolved methods, data analysis, and autonomous experimentation. These efforts build a cross-disciplinary community fluent in dynamic materials science and prepare staff to lead emerging efforts in AI-driven, in situ research.

Outreach and Development

Advancing Goals 5 and 6. Outreach and development efforts form a central pillar of our strategy, particularly regarding Goals 5 and 6. This focus will position CNMS to expand its national impact and recognition while strengthening its role within the broader DOE scientific ecosystem. By proactively engaging partners, enhancing visibility, and aligning our capabilities with emerging national priorities, we will cultivate new opportunities for scientific leadership and user growth. These efforts begin with deeper integration into the SUF Division ecosystem and a renewed commitment to empowering CNMS staff to lead, collaborate, and innovate across institutional boundaries.



STRENGTHEN INTEGRATION INTO THE NATIONAL USER FACILITY ECOSYSTEM

In Goal 5, CNMS is executing a concrete plan to strengthen interactions and coordinate strategically with SNS and HFIR. Outlined in our 90-day response to DOE’s review of the center, included in Appendix C, efforts include road mapping a national deuteration and isotopic substitution resource, co-development of characterization workflows, and a joint Theory–Modeling–AI/ML Hub to connect nanoscale measurements with neutron-scale observables. These actions combined with coordinated staff and user education, joint project planning, and an AI-assisted proposal co-screening tool are poised to facilitate deeper and more meaningful interactions across the facilities.

CNMS also is actively engaging with other NSRCs to leverage collective expertise and understand needs of the centers to refine practices and infrastructure that allow the NSRCs to share AI/ML workflows and expertise. Additionally, working groups around specific capabilities and scientific topics are being developed to coordinate cross-facility workshops and project development teams. Directors at the NSRCs are also working together to understand the opportunities around developing universal user agreements and universal proposals that would formalize cross-facility access for users.

To broaden impact, CNMS is working with ORNL’s Industrial Partnerships and Economic Development groups to refine engagement models, increase presence at industry-focused venues, and adopt metrics that capture collaboration depth (co-development, in-kind contributions, adoption). Detailed milestones and targets for these efforts are also outlined in the 90-Day Response (Appendix C; Recommendation 1) to ensure transparent progress toward increased industrial proposals and partnerships.



FOSTER A THRIVING USER COMMUNITY & STAFF DEVELOPMENT

In Goal 6, CNMS recognizes that the most effective way to foster an engaged and satisfied user community is to first cultivate an engaged and supported staff. To that end, CNMS conducted a series of listening sessions to better understand staff needs, explore concerns, and identify opportunities to improve professional development, communication, and collaboration across the organization. These conversations revealed a deeply committed workforce, with staff who are enthusiastic about scientific opportunities and take great pride in supporting users. At the same time, many expressed challenges in balancing multiple projects and responsibilities.

Sessions tailored to staff at different career stages showed that the CNMS experience differed depending upon time in service. Postdocs and early-career staff had high enthusiasm and passion for science, but they expressed a need for more understanding of operations and basic professional functions, deeper mentorship, and an opportunity to expand their connections and build momentum in their careers. Later-career staff embraced a need to provide quality leadership and mentorship, but they sometimes struggled to balance competing demands between science and leadership roles. Staff at all levels expressed enthusiasm for building a culture of feedback in which constructive criticism and questioning attitudes are more widely embraced as part of day-to-day operations.

To address this input, CNMS is prioritizing tools and processes that streamline communication and scheduling with users, coordinate equipment use across large groups, and improve data sharing and project tracking, ultimately enhancing efficiency, collaboration, and scientific development for staff. Leadership is committed to expanding mentor/mentee opportunities at all career stages and establishing improved onboarding processes to help newer staff move seamlessly into productive work. CNMS is committed to developing techniques and structures to better facilitate constructive feedback and questioning attitudes that can lead to greater insight and engagement.

Overview and Guiding Principles for Investment

CNMS's investment strategy is guided by the dual mission of enabling world-class user science and advancing the forefront of nanomaterials research. Through deliberate planning and prioritization, CNMS has consistently exceeded DOE's 10% recapitalization directive. Leveraging these CNMS operational and capital funds with a combination of Laboratory Directed Research and Development (LDRD) initiatives and Institutional Capital Equipment (ICE) programs, these investments have positioned CNMS as a leader in areas that are directly reflected in, and strengthened by, our three scientific themes (HQM, HCMC, and MD). Together, our groups and themes define the framework through which we identify, develop, and steward the new capabilities needed to address national priorities and meet the evolving needs of the user community.

Our implementation strategy is built around several guiding principles: (1) investing that maintains alignment between user needs and emerging research directions with the CNMS scientific themes, with a strong emphasis on autonomous, data-rich experimentation; (2) maintaining a balance between renewing key capabilities and staff expertise while pursuing transformative new tools and scientific directions; (3) deepening integration across groups through strategic hiring and development of staff whose expertise bridges disciplines; and (4) development of tools, equipment, and capabilities using onsite resources that allow for greater customization and development of staff skills in responding to scientific needs. These principles ensure that our investments sustain operational excellence and also enable the development of new cross-cutting workflows that empower users to engage in multidisciplinary, high-impact research.

Implementation of the CNMS investment plan is an ongoing, adaptive process. Facility improvements and research priorities are informed by the strategic goals of the CNMS and refined through regular assessment of user needs, staff input, and emerging scientific opportunities. The CNMS 5-Year investment plan serves as a living framework, updated annually in consultation with our advisory committees, to reflect changes in priorities, funding, and opportunities for partnership. This dynamic approach ensures that CNMS continues to provide best-in-class instrumentation and expertise, expands its leadership in autonomous and data-driven science, and accelerates the discovery of nanomaterials and phenomena that will define the next generation of energy, quantum, and functional technologies.

Investments and Initiatives Aligned to Strategic Goals



LEAD IN AUTONOMOUS & DATA-DRIVEN NANOSCIENCE

Goal 1 positions CNMS to lead in developing collaborative human-AI workflows that fundamentally reshape how materials research is performed. By tightly integrating synthesis, characterization, modeling, and data analytics into closed-loop, autonomous workflows—and by creating one-of-a-kind experimental platforms that amplify rather than replace scientific expertise—CNMS will accelerate discovery and unlock insights inaccessible through conventional approaches. Achieving this vision requires strategic investment in skilled staff, modern digital infrastructure, and next-generation instrumentation capable of real-time control and multimodal integration. These investments will ensure that CNMS has the people, tools, and platforms necessary to sustain a human-centered, autonomous research ecosystem.

Priority Investments and Initiatives

Expansion of GPU Nodes and Cloud Storage (Near-Term, Annual Investment). To support ML-based force-field development, large-scale simulations, and AI-enabled analysis across CNMS, the center will expand GPU resources by two nodes per year (\$90K per node), targeting a total of eight nodes (16 GPUs). Cloud storage will grow by at least 100 TB per year, with associated internal support (~\$10K/100 TB/year). These investments provide the computational backbone required for closed-loop experimentation and integrated data workflows. This is critical for supporting work across all CNMS strategic goals.

Research Staff with Expertise in Autonomous Workflows (Near- to Mid-Term, Phased Over 3 Years). CNMS will grow its DNA and NTI groups with staff who develop AI-enabled autonomous workflows for STM and electron microscopy (EM) manipulation, information-rich microscopy, and flow-based chemical synthesis. Additional expertise in density functional theory (DFT)/ML-force-field pipeline development will ensure scalable, consistent modeling support across CNMS themes. These hires are essential for enabling predictive control, accelerated discovery, and multiscale integration across Goals 1, 2, 3, and 4.

Instrument Networking (Near-Term, Ongoing Modernization). CNMS, in partnership with ORNL, is deploying 100 Gb connectivity and dedicated instrument-domain networks across laboratories. This infrastructure enables secure, high-bandwidth data streaming from instruments to cloud storage, supporting real-time analysis, autonomous decision making, and multimodal data integration central to human-AI workflows. This is critical to advancing all of CNMS's strategic goals.



UNDERSTAND & UTILIZE HETEROGENEITIES IN QUANTUM MATERIALS

Goal 2 strengthens CNMS's leadership in understanding and harnessing heterogeneities in quantum materials by expanding the capabilities needed to precisely synthesize and assemble low-dimensional systems, identify and control atomic-scale defects and interfaces, and measure their functional behavior in device-relevant settings. Advancing this vision requires tools that can access the structural, electronic, and magnetic degrees of freedom that govern quantum phenomena and can connect local variations in materials to macroscopic performance. By building this integrated suite of synthesis, assembly, and characterization capabilities, CNMS will enable users and staff to transform heterogeneities into a powerful route for designing and validating next-generation quantum architectures and devices.

Priority Investments and Initiatives

Staff Expertise in Scanning Tunneling Microscopy (Near-to Mid-Term). To sustain and expand CNMS leadership in atomic-scale quantum materials characterization, CNMS will recruit a dedicated STM expert to operate and advance the Josephson-Junction STM following the departure of key personnel. This role is essential for developing and maintaining a one-of-a-kind platform that integrates STM with ultra-high-vacuum AFM, enabling simultaneous access to electronic, superconducting, and structural degrees of freedom in quantum and molecular materials. This investment directly supports the core scientific thrust of Goal 2: resolving and controlling heterogeneity at the atomic scale.

Momentum-Resolved, High-Resolution Transmission Electron Microscopy (Mid-Term, 2-3 years, Laboratory Directed Research and Development). CNMS will lead the acquisition and long-term stewardship of a momentum-resolved high-resolution transmission electron microscope (TEM). This instrument will provide capabilities that bridge neutron and X-ray scattering with real-space imaging, enabling direct correlation between electronic excitations, collective modes, and atomic-scale structure that are central to quantum materials' function. CNMS will maintain service contracts, provide expert staffing, and expand the system with cryogenic holders to support quantum-relevant measurements, also impacting Goals 4 and 5.

Upgraded Low-Dimensional Materials Handling Glovebox Infrastructure (Near-Term, 1-2 years). To enhance the synthesis, transfer, and device integration of 2D and heterostructure materials, CNMS will continue upgrades to its low-dimensional materials nanofab-in-a-glovebox facility. Additions will include an upgraded probe station for device-level functional characterization, an AFM for topographic and thickness mapping, and vacuum suitcase to allow for sharing air-sensitive low-D materials. These upgrades are critical to maintaining a safe, efficient, contamination-free environment for the preparation and multi-modal characterization of high-quality quantum materials and moiré heterostructures.

Arbitrary Waveform Generator and RF Control Platform for Electron Spin Resonance STM (Near-Term, 1-2 years). Goal 2 requires the ability to probe and manipulate spin dynamics at the single-atom level. CNMS will invest in an arbitrary waveform generator and a unified RF control platform for the development of electron spin resonance (ESR)-STM, enabling synchronized control of RF fields, STM operation, and spin-dependent characterization in controlled magnetic field environments. These capabilities will allow measurement and manipulation of spin dynamics in single atoms and molecules at nanosecond timescale, essential for coherent spin manipulation, spin-resolved spectroscopy, and exploring defect- and heterogeneity-driven quantum behavior.



HARNESS COMPLEX MACROMOLECULAR CONFORMATIONS

Goal 3 strengthens CNMS's leadership in soft matter and hybrid materials by enhancing the capabilities needed to understand and control how macromolecular conformations evolve under electrostatic, topological, and processing-driven forces. Predictive control of polymer behavior—particularly at soft-hard interfaces and in non-equilibrium settings—requires the ability to synthesize high-purity materials, probe their multiscale structure with high chemical sensitivity, and link these features to functional performance. By expanding synthesis capacity, analytical chemistry, and advanced chemical imaging, CNMS will more effectively map chain conformation, interfacial organization, and metastable structures, positioning the center to design polymer systems that overcome traditional performance trade-offs and enable next-generation membranes, actuators, composites, and functional soft materials.

Priority Investments and Initiatives

Expanded Staffing in Analytical Chemistry and Chemical Synthesis (Near- to Mid-Term, 1-3 years).

To support the growing demand for high-quality polymer synthesis, deuterated materials, and soft-matter characterization, CNMS will invest in additional staffing for analytical chemistry and chemical synthesis. A dedicated analytical chemistry technician will increase instrument uptime, ensure reliable purification and validation workflows, and expand access to critical capabilities utilized by both users and thematic research teams. Adding a technical professional in chemical synthesis will broaden CNMS's capacity to prepare advanced materials, including deuterated polymers and small molecules, directly supporting CNMS users and enhancing collaboration with SNS and HFIR for neutron-based soft-matter studies.

Modernization of Analytical Instrumentation for Polymer and Small-Molecule Characterization (Near-Term, 1-2 years).

To replace aging equipment and enrich the depth of chemical and structural information available for HCMC studies, CNMS will invest in a suite of updated analytical tools. Planned acquisitions include a benchtop nuclear magnetic resonance (NMR) system, dynamic light scattering instrumentation, an impedance analyzer, and ellipsometry tools. These instruments are essential for quantifying polymer conformations, chain dynamics, film behavior, and electrostatic interactions—core elements of the HCMC research paradigm. Updating this infrastructure is

critical to sustaining complementary workflows with SNS/HFIR (Goal 5) and reducing staff time spent on troubleshooting aged equipment (Goal 6).

Enabling Advanced Chemical Imaging of Soft Matter with Atom Probe and Correlative Tools (Mid-Term, 3-5 years). CNMS, leveraging the Major Items of Equipment (MIE) Recapitalization project and ORNL Institutional Capital Investment, has invested in cryo-EM, cryo-Atom Probe Tomography (APT), and a cryo-enabled plasma focused ion beam (FIB), establishing a foundation for studying liquid/solid interfaces and nanoscale chemical analysis that is rarely accessible for soft matter. Additional investments to enable controlled preparation and cryogenic transfer of soft-matter samples across modalities will enable quantitative 3D compositional mapping of polymer interfaces, electrostatic architectures, and hybrid systems. Complementary upgrades, including a time-of-flight secondary ion mass spectrometry (ToF-SIMS) attachment for the Helios Hydra, will provide high-resolution chemical imaging and cross-sectioning, supporting correlative workflows that link nanoscale chemistry to macroscopic function. Together, these tools will substantially expand CNMS's ability to interrogate and design complex macromolecular systems and strengthen connections to soft-matter and biological research across the SUF Division ecosystem (Goal 5).



DIRECT MULTISCALE DYNAMICS & TRANSFORMATIONS

Goal 4 advances CNMS's ability to understand, predict, and control how energy flows and transforms materials across the atomic-to-device hierarchy—capabilities essential for next-generation microelectronics, quantum devices, and integrated fabrication processes. Achieving this vision requires tools that can synthesize materials under precisely tuned non-equilibrium conditions, probe ultrafast and nanoscale excitations, and track structural and chemical evolution in real time. By expanding autonomous synthesis platforms, enhancing electron- and optical-based spectroscopies, and modernizing imaging systems for automated and AI-guided analysis, CNMS will create an integrated environment for revealing how defects, interfaces, and collective excitations govern functional performance. These investments will equip CNMS to intentionally steer material transformations and to accelerate the discovery of architectures that deliver new levels of speed, efficiency, and quantum functionality.

Priority Investments and Initiatives

Automated Synthesis and Processing Chamber V3.0 (Near-Term, 1-2 years). CNMS will develop a V3.0 automated synthesis and characterization chamber that builds on earlier autonomous platforms and unifies pulsed laser deposition, direct current sputtering, and an RF ion source to enable controlled thin-film growth and irradiation in a single platform. The system will collect real-time structural, chemical, and optical data during synthesis and processing, enabling autonomous, AI/ML-driven optimization of growth conditions and defect-function relationships. Fully integrated into CNMS and ORNL data networks, the platform will accelerate discovery in quantum materials, microelectronics, and radiation-tolerant systems while providing high-quality datasets for digital twin and predictive modeling efforts. This effort is crosscutting for Goals 1, 2, and 5.

Expansion of SEM-CL Capabilities and Dedicated Staff Support (Near-Term, 1-2 years). To deepen nanoscale optical and electronic characterization, CNMS will expand its scanning electron microscopy–cathodoluminescence (SEM-CL) system by adding a UV-sensitive detector capable of measurements down to 200 nm. A full-time staff member will be hired to maintain the system, support users, and broaden CNMS’s optical spectroscopy portfolio, directly benefiting research on excitations, recombination pathways, and defect-driven functionality in electronic and quantum materials.

Replacement and Modernization of SEM for Automated and Autonomous Imaging (Mid-Term, 2-3 years). CNMS will replace an aging SEM with an updated system that offers significantly faster imaging, improved stability, and advanced automation. This new platform will enable autonomous feature identification, high-throughput imaging workflows, and algorithm-guided search routines—advancing the center’s capabilities in identifying defects, interfaces, and dynamic transformations at device-relevant scales.

Advancement of Time-Resolved THz and Functional AFM Capabilities (Mid-Term, 3-4 years). CNMS will invest in a time-resolved THz time-domain spectroscopy AFM to probe ultrafast carrier dynamics, phonons, plasmons, and polaritons at the nanoscale. This capability will provide unique insight into energy flow and collective excitations in materials relevant to 6G microelectronics and emerging quantum technologies. Expanding functional AFM platforms will enable users to interrogate dynamic processes with unprecedented spatiotemporal resolution, strengthening both user-driven science and CNMS thematic research.



STRENGTHEN INTEGRATION INTO THE NATIONAL USER FACILITY ECOSYSTEM

Goal 5 reinforces CNMS’s commitment to functioning as a connected, collaborative contributor within the national user facility ecosystem. Strengthening these connections requires not only scientific coordination but also modernized digital infrastructure, enhanced user engagement, and streamlined pathways that enable seamless access across SUF Division facilities. The investments outlined in Goals 1–4 will expand CNMS’s unique capabilities in synthesis, characterization, and autonomous workflows, positioning the center to generate and share the high-value, multi-modal datasets that are essential for cross-facility collaboration and the Genesis platform vision. By improving proposal systems, expanding outreach, and deploying AI-enabled tools that help users navigate capabilities and workflows across CNMS, SNS, HFIR, and the NSRCs, CNMS will broaden its scientific reach and enable more efficient, integrated discovery. These efforts will ensure that CNMS remains an accessible, collaborative, and high-impact resource for the national research community.

Priority Investments and Initiatives

Enhancement of Digital User Interfaces and Proposal Systems (Near-Term, 1-2 years). CNMS will update its user-facing digital interfaces to streamline proposal submission across facilities,

enhance equipment scheduling, and improve project tracking. This effort includes redesigning the web-based proposal platform to provide a clearer view of CNMS capabilities, reduce administrative burden, and better support users navigating multi-facility workflows with SNS, HFIR, and other NSRCs.

AI-Enabled Proposal Screening and Capability Matching (Near-Term, 1-3 years). To improve user support and help researchers find the most relevant tools and expertise, CNMS will develop AI-enabled systems that analyze proposal content, identify required capabilities, and recommend complementary resources across CNMS and partner facilities. This capability will enhance cross-facility coordination and help users build more effective experimental plans.

Strengthened Outreach and Cross-Facility Engagement (Near-Term, Ongoing). CNMS will expand targeted outreach to academic, industry, and government institutions through webinars, workshops, cross-facility open houses, and direct engagement with emerging research communities. These efforts will highlight CNMS signature capabilities in soft matter, quantum materials, and autonomous workflows while enabling new users to better integrate neutron scattering, modeling, and other SUF Division capabilities into their research.

Integration of Efforts Identified in the CNMS 90-Day Response (Near- to Mid-Term, as described). As outlined in the 90-day response, CNMS will continue efforts to develop shared data standards, coordinate deuteration and synthesis workflows with SNS/HFIR, and create pathways for interoperable data, sample provenance, and multimodal analysis. These initiatives will improve the user experience and strengthen CNMS's role as a contributor within a more unified SUF Division research ecosystem.



FOSTER A THRIVING USER COMMUNITY & STAFF DEVELOPMENT

Goal 6 strengthens CNMS's long-term impact by investing in the people and systems that make collaborative, multidisciplinary research possible. As user projects increasingly involve autonomous workflows, multimodal characterization, and cross-facility integration, CNMS must equip staff with the training, tools, and resources needed to support these complex efforts. By expanding staffing, enhancing digital and data infrastructure, and improving communication pathways, CNMS will create an environment where staff can develop new skills, work more efficiently, and deliver exceptional support to users. These investments will elevate the effectiveness of user engagement, broaden outreach to academic and industrial partners, and cultivate a dynamic workforce capable of leading and adapting as scientific needs evolve.

Priority Investments and Initiatives

Targeted Outreach and Communication Support (Near-Term, 1-2 years). CNMS will partner with ORNL communications and industrial partnerships offices and leverage resources to improve outreach materials and web content, ensuring that users, especially from industry, can easily

understand available capabilities and how to engage with the center. Clearer communication also strengthens staff capacity by reducing redundant inquiries and enabling more efficient user interactions.

Structured Onboarding and Mentoring Programs (Ongoing). Regular quarterly onboarding sessions and formal mentoring programs will help new and current staff understand CNMS workflows, scientific themes, and cross-facility opportunities. These programs will support career development, foster collaboration, and ensure that staff are well prepared to guide users through advanced research environments.

Enhanced Data Systems for User Interaction and Project Tracking (Near-Term, 1-3 years). Modernizing digital systems that track user interactions, project progress, and scheduling will streamline staff workflows and reduce administrative burden. These interfaces will centralize information, improve communication, and eventually incorporate AI/ML tools to recommend capabilities, flag bottlenecks, and optimize resource allocation, enhancing both user experience and staff efficiency.

Professional Development for Multidisciplinary Research Support (Ongoing). CNMS will expand training in data-driven research, autonomous experimentation, neutron and multimodal workflows, and user engagement best practices. This investment ensures staff remain agile and prepared to assist users in cutting-edge research contexts while broadening their own scientific and technical competencies.

Risk Identification and Mitigation

CNMS maintains a proactive and structured approach to identifying, assessing, and mitigating operational risks to ensure safe, reliable, and sustainable user facility operations. Risk identification and mitigation are embedded in routine leadership and operational processes through regular meetings that include group leaders, section heads, user program management, and operations staff. These structured discussions—combined with direct engagement between leadership, staff, and users—allow early identification of potential issues. Observations and concerns are captured in the ORNL “Insights” system to ensure transparency, accountability, and continuous tracking. High-priority risks are elevated promptly to ORNL and DOE leadership, where mitigation actions are coordinated across organizational and facility boundaries. CNMS conducts and evaluates user surveys annually and has engaged the user executive committee to conduct one-on-one interviews with users to help develop best-practice guidelines and recommendations for interfacing with users.

Operational risks in recent years have included supply chain constraints—such as helium expense and availability—increased delivery times for equipment procurement, aging infrastructure and equipment, staffing and retention challenges, and rapidly evolving funding environments. Mitigation strategies are designed to maintain both operational continuity and scientific excellence. CNMS has implemented helium recovery and recycling systems, established preferred vendor agreements, and strengthened maintenance planning to address supply challenges. Targeted hiring, mentoring, and individualized development planning efforts are aimed at sustaining critical expertise, while proactive equipment recapitalization and service contracts ensure high instrument uptime and reliable user support. Lessons learned from realized risks are routinely discussed in leadership meetings, captured in the Insights system, and shared across facilities to improve processes and reinforce best practices.

Looking forward, CNMS’s risk mitigation strategy focuses on the following principles:

Mission-driven prioritization: Risk mitigation actions are evaluated by their impact on safety, user program continuity, and scientific productivity, ensuring the most critical issues are addressed first.

Structured and transparent processes: Regular leadership meetings, direct staff and user engagement, and the ORNL Insights system ensure consistent identification, communication, and tracking of risks.

Dual-value investments: CNMS directs resources toward actions that stabilize current operations and enable future innovation, balancing near-term reliability with long-term advancement.

Strategic workforce development: Targeted hiring, mentoring, and early-career integration safeguard critical expertise and build next-generation leaders in key research and technical areas.

Phased implementation: When resources are limited, upgrades and mitigations are executed in phases to maintain uninterrupted user access while progressively strengthening facility capability and infrastructure.

Metrics and Timelines

CNMS operates as a DOE SC user facility dedicated to advancing nanoscience through open access, cutting-edge capabilities, and multidisciplinary collaboration. Effective governance and transparent performance metrics are essential to ensuring scientific excellence, responsible stewardship, and user impact. Our approach emphasizes measurable progress toward strategic goals, continuous evaluation, and adaptive management.

Metrics and Tracking Progress

CNMS will employ a comprehensive suite of metrics to evaluate scientific output, user impact, and operational effectiveness. Core scientific metrics will continue to include the number of publications generated by CNMS staff and users, along with the percentage appearing in high-impact journals (impact factor greater than 7). User program metrics will track the number of unique users, distribution of on-site versus remote access, percentage of first-time users, and user satisfaction as assessed through the annual survey. These data will be complemented by detailed demographic and institutional information, including user type (academic, government, industry), researcher career stage, citizenship, state-level distribution of domestic users, funding mechanisms, and research categories, allowing CNMS to understand and broaden its reach across disciplines, institutions, and communities.

Operational and programmatic effectiveness will also be monitored through project-level reporting, including the number of active projects, institutional and funding breakdowns, and publication types (user-led, CNMS-led, and collaborative). These quarterly assessments provide a near-real-time view of activity levels across the center and highlight evolving trends in user engagement, scientific productivity, and industrial participation.

To support modern workflows and ensure the reliability of critical instrumentation, CNMS will implement a new logging system that tracks instrument scheduling, tool use, maintenance intervals, development activities, and downtime. These metrics will provide an objective basis for assessing instrument performance, allocating technical support, identifying bottlenecks, and prioritizing recapitalization or modernization efforts. Over time, these data will also support AI-enabled operational analytics that help optimize instrument availability, improve user scheduling, and enhance long-term planning for maintenance and equipment development. These analytics even open the door to providing AI-enabled experimental guidance and recommendations to users about what additional tools can be harnessed to augment their work. Together, these metrics will give CNMS a robust, data-driven foundation for evaluating progress toward its strategic goals, improving the user experience, and sustaining operational excellence.

Review and Refresh Cycle

CNMS will conduct an annual meeting with the User Executive Committee and Scientific Advisory Committee to conduct a review of progress toward our strategic objectives. Assessments will be conducted of both progress and validity of objectives based on evolving priorities. Appropriate revisions will be made based on feedback from the advisory committees. Commensurate with DOE reviews, scientific themes and investment priorities will be reviewed and revised, informed by user feedback, advisory input, and emerging national priorities. Adjustments will be codified in an updated 5-year implementation plan.

Reporting, Transparency, and Improvement

CNMS will maintain transparent reporting mechanisms to ensure accountability and learning. A public-facing annual report will summarize user statistics, scientific highlights, and progress toward strategic goals. Internally, CNMS will track operational metrics (uptime, utilization, cost recovery, safety) and scientific outcomes (publications, partnerships, awards) and use these metrics to inform decisions about investments in staff and new capabilities. Feedback from the User Executive Committee and Scientific Advisory Committee will directly inform mid-course corrections. Continuous improvement will be embedded through regular after-action reviews, user surveys, and data-driven decision processes.

Conclusion

Following the successful completion of this strategic plan, the Center for Nanophase Materials Sciences will emerge as a model for how modern science is conducted, integrating human expertise, autonomous experimentation, advanced computation, and one-of-a-kind instrumentation into a seamless engine for discovery that supports national priorities. CNMS will be recognized as a leader in human-AI scientific collaboration, with autonomous and data-driven workflows routinely accelerating the pace of materials synthesis, characterization, and modeling. Scientists and users will work together within tightly coupled feedback loops that reveal materials behavior across scales, producing insights and capabilities that would have been inaccessible through traditional approaches.

In quantum materials, soft matter, and dynamic functional systems, CNMS will have transformed heterogeneity, non-equilibrium behavior, and structural evolution into controllable design parameters. These discoveries will provide the scientific foundations for next-generation quantum devices, advanced polymers, and energy-efficient microelectronics. User access to these advances will be frictionless, supported by a staff whose expertise, training, and multidisciplinary collaboration ensure exceptional scientific engagement and impact. The center's investment in professional development, AI-enabled user support, and modernized operational practices will solidify CNMS as a model environment for scientific excellence and community building.

As an increasingly integrated member of the national user facility ecosystem, CNMS will contribute high-value multimodal datasets, interoperable workflows, and shared capabilities that amplify the collective strength of the NSRCs, neutron sources, light sources, and high-performance computing centers. The center will continue to serve as a gateway to neutron science through deuteration, advanced characterization workflows, and theory-modeling partnerships, enabling users to tackle problems of national importance with unprecedented depth and resolution.

Five years from now, CNMS will stand as a hallmark of the nation's scientific ecosystem, a place where new ideas become new materials, where new materials become new technologies, and where a vibrant user community collaborates with an empowered staff to advance the energy, economic, and national security priorities of the United States.

Appendix A: Abbreviations

AI	artificial intelligence
AFM	atomic force microscopy
APT	atom probe tomography
BES	Office of Basic Energy Sciences
BRN	Basic Research Needs
CNMS	Center for Nanophase Materials Sciences
DFT	density functional theory
DOE	U.S. Department of Energy
DRE	digital research environment
EM	electron microscopy
FIB	focused ion beam
FAIR	Findable, Accessible, Interoperable, Reusable
HFIR	High Flux Isotope Reactor
ICE	institutional capital equipment
LDRD	Laboratory Directed Research and Development
ML	machine learning
NSRC	Nanoscale Science Research Center
OLCF	Oak Ridge Leadership Computing Facility
ORNL	Oak Ridge National Laboratory
QCM	quartz crystal microbalance
QIS	quantum information science
RF	radio frequency
SC	Office of Science
SEM	scanning electron microscopy
SNS	Spallation Neutron Source
STM	scanning tunneling microscopy
SUF	Scientific User Facilities

CNMS Science Themes:

HCMC	Harnessing Complex Macromolecular Conformations
HQM	Heterogeneities in Quantum Materials
MD	Multiscale Dynamics

CNMS Groups:

DNA	Data NanoAnalytics
eMMA	electron Microscopy and Microanalysis
F-AFM	Functional Atomic Force Microscopy
FHN	Functional Hybrid Nanomaterials
MACRO	Macromolecular Nanomaterials
NRL	Nanofabrication Research Laboratory
NTI	Nanomaterials Theory Institute
STM	Scanning Tunneling Microscopy

Appendix B: CNMS Group Summaries

electron Microscopy and Microanalysis (eMMA) Group

Website: <https://www.ornl.gov/group/electron-microscopy-and-microanalysis>

Core Expertise: The eMMA group pioneers advanced electron beam imaging and spectroscopy methods as well as atom probe tomography to reveal the fundamental structure-property-function relationships that underpin materials behavior.

Signature Capabilities:

- *Aberration-corrected Scanning Transmission Electron Microscopy* for atomic-resolution structural imaging and spectroscopy
- *High-energy-resolution electron energy loss spectroscopy (EELS)* to probe vibrational, optical, and electronic excitations with temperature control
- *Cryogenic electron microscopy and specimen preparation* for imaging beam-sensitive, soft, quantum, and biological materials at near-atomic resolution
- *In situ and operando microscopy* under diverse environmental conditions (liquid, gas, vacuum) and external stimuli (temperature, pressure, electrical bias, and optical excitation)
- *Lorentz and phase-contrast imaging* to resolve nanoscale magnetic textures and dynamic field responses
- *APT* for three-dimensional chemical mapping at sub-nanometer resolution

Alignment with Strategic Goals:

The eMMA group serves as a nexus for atomic-to-mesoscale structural and chemical characterization across the CNMS science themes.

Goal 1 (Autonomous and Data-Driven Discovery) – eMMA anchors CNMS’s multimodal characterization ecosystem, linking nanoscale imaging with AI/ML analytics (DNA), theoretical modeling (NTI), and fabrication workflows (NRL).

Goal 2 (Heterogeneities in Quantum Materials) – eMMA provides high-resolution imaging and spectroscopy to correlate local atomic structure and defects with emergent quantum phenomena, while providing a foundation for next-generation platforms for atomic manipulation.

Goal 3 (Harness Complex Macromolecular Conformations) – eMMA contributes cryo-EM expertise to probe soft, hybrid, and biological nanostructures.

Goal 4 (Multiscale Dynamics) – eMMA’s operando and cryo capabilities enable real-time visualization of phase transformations, reactions, and dynamic processes.

Goal 5 (User Facility Integration) – Emerging techniques in electron scattering and Lorentz microscopy provide a powerful complement to neutron scattering capabilities at SNS and HFIR.

Functional Atomic Force Microscopy (F-AFM) Group

Website: <https://www.ornl.gov/group/functional-atomic-force-microscopy>

Core Expertise: The F-AFM group advances ambient scanning probe microscopies and spectroscopies to capture the nanoscale origins of functional properties in materials. The team develops novel approaches to use the probe tip as a localized source of strain, electric, magnetic, optical, and thermal fields, while simultaneously detecting the corresponding responses through high-sensitivity measurements with high spatial precision, integrated with AI-enhanced data acquisition and analysis.

Signature Capabilities:

- Advanced data acquisition and control systems for synchronized delivery of tip-induced excitation and detection of complex electrical, optical, and thermal stimuli
- Multifrequency and user-directed scanning probe trajectories to enable rapid and efficient material manipulation and AI-driven workflows
- AI/ML-assisted imaging, spectroscopy, and data analysis in collaboration with the DNA Group
- Integration of optical spectroscopy with scanning probe microscopy for correlative photoresponse measurements

Alignment with Strategic Goals:

Goal 1 – F-AFM integrates advanced control and AI-enabled analysis in concert with the DNA group to accelerate data acquisition, interpretation, and autonomous experimentation in scanning probe platforms.

Goal 2 – Provides nanoscale electromechanical and optical probes of quantum and correlated materials, revealing how local fields and strain influence emergent phenomena

Goal 3 – Explores nanoscale mechanical and electrical behavior in soft, hybrid, and polymeric materials to link local conformation with macroscopic function

Goal 4 – Delivers real-time, multimodal measurements of dynamic processes such as domain switching, transport, and structural transformations

Goal 5 – F-AFM offers unique multimodal scanning probe capabilities that complement electron microscopy (eMMA) and neutron scattering (SNS, HFIR), enabling correlative studies that link nanoscale defects to macroscale behavior in polarizable, magnetic and electronic materials. The group is also emerging as a resource for measuring swelling from local conformational changes in soft matter systems.

Scanning Tunneling Microscopy (STM) Group

Website: <https://www.ornl.gov/group/scanning-tunneling-microscopy>

Core Expertise: The STM group develops and applies advanced scanning tunneling microscopy and spectroscopy techniques to understand and control the correlations between atomic structure, electronic behavior, and magnetic and transport properties in quantum materials. The team focuses on revealing and manipulating quantum states and interactions at the atomic scale to tailor emergent phenomena in low-dimensional systems.

Signature Capabilities:

- Atomic-resolution imaging, electronic density-of-states mapping, and nanoscale electron transport measurements in quantum materials
- Dilution-refrigerator vector magnet STM enabling imaging and spectroscopy from 40 mK to 300 K and magnetic fields up to 9 T
- Spin-polarized four-probe STM, allowing spatially resolved transport and spin-sensitive measurements
- AI-integrated workflows for the construction and measurement of electronic states in atomic arrangements
- Room-temperature and cryogenic-temperature scanning nitrogen-vacancy (NV) center microscopes for magnetic and quantum sensing with nanoscale resolution

Alignment with Strategic Goals:

Goal 1 – Develops, maintains, and implements autonomous experiments coupling STM spectroscopy and atomic manipulation workflows

Goal 2 – Enables direct visualization and manipulation of correlated electron behavior, spin textures, and topological excitations to connect atomic defects and local electronic structures with emergent quantum behavior

Goal 3 – Combines controlled on-surface chemical reactions and in situ molecular level imaging to inform the precision synthesis of organic framework and interfaces

Goal 4 – Investigates time-dependent electronic and magnetic fluctuations at the atomic scale to connect local dynamics to macroscopic properties

Goal 5 – Links neutron-resolved long-range order with nanoscale structural and electronic variations to provide comprehensive insight into emergent quantum functionalities.

Macromolecular Nanomaterials (MACRO) Group

Website: <https://www.ornl.gov/group/macromolecular-nanomaterials>

Core Expertise: The MACRO group designs and synthesizes novel macromolecular and deuterated nanomaterials to understand and control nanophase behavior in soft matter systems. By combining advanced synthetic chemistry, state-of-the-art characterization, and computational modeling across atomistic to coarse-grain scales, the group seeks to reveal the molecular origins of complex soft-matter phenomena and guide the design of next-generation functional polymers and hybrid materials. A central mission of the group is to develop tailored, deuterated macromolecules as well as complementary characterization techniques that are tightly coupled to neutron-based investigations at SNS and HFIR.

Signature Capabilities:

- Deep integration of soft matter and hybrid materials science with neutron scattering
- Precision synthesis of tailored and deuterated small molecules, polymers, and bio-derived macromolecules
- Advanced continuous-flow polymerization and reaction monitoring integrated with AI/ML-driven feedback and optimization
- Comprehensive soft-material characterization tools, enabling detailed thermal, mechanical, and dynamic property analysis
- Synergistic combination of experimental data with multiscale modeling and simulations from atomistic to coarse-grained

Alignment with Strategic Goals: The MACRO group anchors CNMS expertise in soft and hybrid materials and provides complementary capabilities and critical material support that are deeply integrated with neutron-enabled research.

Goal 1 – Accelerates polymer design and synthesis by implementing AI/ML-enabled workflow and operando monitoring in continuous flow reactors

Goal 2 – Contributes to understanding of hybrid systems where polymeric interfaces influence functional properties in a significant manner

Goal 3 – Leads CNMS efforts to design, synthesize, and characterize macromolecules with controlled architectures and responsive functions

Goal 4 – Enables multi-scale modeling of macromolecules by generating experimental results across a broad range of length and time scales

Goal 5 – Grows precision synthesis of deuterated and polymeric materials and complementary characterization capabilities that are deeply embedded with neutron scattering research at SNS and HFIR

Nanofabrication Research Laboratory (NRL) Group

Website: <https://www.ornl.gov/group/nanofabrication-research-laboratory>

Core Expertise: The NRL group advances nanofabrication processes to evoke and elucidate the effects of scale and confinement on the function of nanomaterials and soft matter. The group leverages semiconductor processing and direct-write techniques to translate materials discoveries into functional nanoscale and microscale architectures that enable discovery of novel material behavior. Research focuses on understanding and controlling material transformations and defect formation that occur during patterning and energetic processing to understand their fundamental role in functional systems critical to sensing, information processing, and next-generation microelectronics. The team supports a 10,000 sq ft. clean room with a comprehensive suite of capabilities for nanofabrication.

Signature Capabilities:

- Direct-write fabrication via reactive and inert FIB, e-beam–induced chemistry, and two-photon polymerization for rapid 3-D prototyping and nanoscale material modification
- Integration of top-down and bottom-up fabrication methods to merge soft matter, hybrid, and inorganic materials into functional devices and microfluidics platforms
- Foundational research on ion- and electron-beam-induced chemistry to understand nanoscale material manipulation and defect engineering with energetic beams

Alignment with Strategic Goals: The NRL provides the fabrication and integration foundation that links CNMS’s materials discoveries to functional systems and devices.

Goal 1 – NRL is working toward adapting nanofabrication tools for AI/ML-guided direct-write materials synthesis, low-damage etch methods, and systematic defect engineering.

Goal 2 – NRL is pioneering the development of *in situ* integrated materials interrogation platforms that reveal novel atomic scale processes and emergent quantum behavior.

Goal 3 – The group leads efforts in tailoring surface structure and chemistry to integrate soft and hybrid materials into engineered architectures.

Goal 4 –NRL develops precise nanofabricated platforms that facilitate measurement of electronic and optical properties of layered 2D materials.

Goal 5 – NRL is the center for advanced research and development on diamond stripper foils that support neutron production. Staff work with SNS/HFIR to shape fluidic chambers for in situ liquid reflectometer processes and tailored interfaces that support measurements of lipid bilayer memristors.

Functional Hybrid Nanomaterials (FHN) Group

Website: <https://www.ornl.gov/group/functional-hybrid-nanomaterials>

Core Expertise: The FHN group focuses on designing and synthesizing novel functional materials that address emerging quantum, energy, and microelectronic applications. A key focus is developing and implementing in situ and operando diagnostics to monitor and guide materials synthesis and processing through automated workflows.

Signature Capabilities:

- Growth and processing of single crystal thin films and 2-D materials using pulsed laser deposition (PLD), sputtering, CVD, exfoliation, and controlled environmental transfer and stamping techniques
- Low energy light ion implantation and irradiation studies with operando multimodal characterization
- In situ and operando optical spectroscopy for monitoring structure and functionality during synthesis or external stimulation
- Autonomous PLD systems incorporating in situ reflection high-energy electron diffraction (RHEED), X-ray photoelectron spectroscopy (XPS), X-ray fluorescence (XRF), Raman, and advanced data acquisition for scientist-in-the-loop synthesis and growth model development
- “Lab-on-a-crystal” QCM platforms integrating electrical, optical, and gravimetric/viscoelastic measurements with AI/ML-driven data analysis
- Ultrafast laser micro-spectroscopy for probing quasiparticle and carrier dynamics in 2-D materials and heterostructures
- Linear and nonlinear optical spectroscopy, including micro-absorption, photoluminescence (PL), PL lifetimes, and second harmonic generation (SHG) for characterization of low-dimensional quantum materials
- Cathodoluminescence spectroscopy with nanometer resolution, coupled to single superconducting nanowire photon detection, for quantum emitter characterization

Alignment with Strategic Goals:

Goal 1 – Pioneers AI/ML-integrated, closed-loop synthesis workflows using in situ diagnostics and automated data acquisition for smart materials growth

Goal 2 – Develops and studies 2-D and hybrid quantum materials where structure, strain, and composition control electronic, optical, and spin phenomena

Goal 3 – QCM platforms provide deep understanding of soft material behavior and response at interfaces. AI/ML driven synthesis discoveries are being translated to autonomous chemistry platforms

Goal 4 – Uses in situ spectroscopy and ultrafast techniques to track nonequilibrium dynamics and phase transitions in 2-D materials and thin films

Goal 5 – Closely integrating with SNS and HFIR to develop characterization workflows to complement time-resolved reflectometry and scattering characterization of quantum and magnetic materials

Nanomaterials Theory Institute (NTI) Group

Website: <https://www.ornl.gov/group/nanomaterials-theory-institute>

Core Expertise: The NTI group delivers advanced theoretical, computational, and ML capabilities that underpin the fundamental understanding and prediction of materials behavior and chemical processes at the nanoscale. NTI connects theory and simulation with experiment to interpret, predict, and steer the discovery of novel quantum, soft, and energy-relevant materials.

Signature Capabilities:

- Multiscale modeling platforms covering quantum (DFT, beyond-DFT), atomistic (MD, MC), coarse-grained, and continuum approaches for structure-property prediction
- AI/ML-driven materials modeling for surrogate modeling, uncertainty quantification, and accelerated exploration of structure-function relationships
- Predictive simulations of strongly correlated materials, nanoscale transport, and nonequilibrium processes under external fields
- Large-scale simulations of soft matter, interfaces, and hybrid systems, including polymer and biomolecular assemblies
- Development and application of scalable codes for exascale computing, with dedicated access to CNMS's internal clusters and DOE leadership computing resources
- Collaborative integration of theory and experiment to interpret spectroscopy, microscopy, and scattering data from CNMS, SNS, and HFIR

Alignment with Strategic Goals:

Goal 1 – Leads development of AI/ML-integrated modeling workflows that combine data from simulations and experiments for predictive materials design

Goal 2 – Predicts and explains emergent phenomena in correlated and topological materials, including spin, charge, and lattice interactions

Goal 3 – Models multiscale structure and dynamics of polymers and hybrid materials to link molecular design with functional performance

Goal 4 – Simulates real-time evolution of structural, magnetic, and electronic processes and structural changes from beam material interactions to bridge atomic- to mesoscale behavior

Goal 5 – Provides computational resources and expertise to CNMS and neutron facility users and collaborates with neutron scattering facilities (SNS, HFIR) to interpret experiments and guide new measurements

Data NanoAnalytics (DNA) Group

Website: <https://www.ornl.gov/group/data-nanoanalytics>

Core Expertise: The DNA group accelerates the development of autonomous research tools and workflows for nanoscale synthesis and characterization by integrating physics-driven ML, simulations, and instrument automation. DNA's efforts transform CNMS instruments into intelligent research platforms with humans in the loop capable of learning, adapting, and driving new types of experiments that seamlessly integrate computation, characterization, and synthesis.

Signature Capabilities:

- Physics-informed ML models for multimodal data streams enabling high-fidelity reconstruction and analysis of nanoscale phenomena
- Closed-loop, autonomous experimental workflows that integrate ML algorithms with simulations, digital twins, and real-time instrument control for characterization and synthesis
- Edge-computing and cloud-based infrastructure for real-time and ad-hoc data processing and feedback to experimental systems
- AI-assisted imaging, spectroscopy, and control for deterministic atomic and mesoscopic manipulation, phase transformations, and growth optimization of functional materials
- Development of open-source and user-accessible tools for analysis, automation, and data standardization to extend autonomous science capabilities to the broader CNMS user community

Alignment with Strategic Goals:

The DNA group serves as the digital and analytical backbone of CNMS, enabling autonomous, data-rich discovery across all scientific themes.

Goal 1 – Leads CNMS efforts in AI/ML-enabled autonomous science, combining instrument automation, physics-informed learning, and simulations to accelerate discovery

Goal 2 – Applies ML-driven data analysis for automated microscopy to reveal and manipulate defects and topological structures governing emergent quantum behavior

Goal 3 – Develops data pipelines and LLMs to steer chemical reactions in autonomous chemistry platforms

Goal 4 – Implements real-time analytics and feedback control to study phase transitions and material responses under external stimuli

Goal 5 – Builds and maintains the data infrastructure, edge computing, and AI/ML frameworks that link CNMS instruments, theory, and neutron facilities, empowering users with next-generation data-driven workflows

Appendix C:

90-Day Response to BES-SUFD Quinquennial Operations Review of the Center for
Nanophase Materials Sciences

September 25, 2025

Dr. Mikhail Zhernenkov
Program Manager, Scientific User Facilities Division
Office of Basic Energy Sciences
U.S. Department of Energy
19901 Germantown Road
SC-22.3; E-402
Germantown, Maryland 20874-1290

Dear Dr. Zhernenkov:

90-Day Response to BES-SUFD Quinquennial Operations Review of the Center for Nanophase Materials Sciences (CNMS)

This letter represents the 90-day response to the three Action Items and one Recommendation provided by the Office of Basic Energy Sciences (BES) Scientific User Facilities Division (SUFD) in the letter received on June 26, 2025, following the 5-year Operations Review of the Center for Nanophase Materials Sciences (CNMS). The review was held at the Oak Ridge National Laboratory (ORNL) on April 30 – May 1, 2024, and covered operation of the facility, research activities during fiscal years (FYs) 2019-2023, as well as future plans for the Center.

We would like to thank BES for their organization of the review meeting as well as the members of the review panel for their time and thoughtful evaluation of the CNMS user and research programs, and for providing a comprehensive and constructive review. We are pleased that the Center was recognized for its overall effectiveness and for having a dedicated staff who produce impactful publications and foster a productive user program within a supportive environment.

Staff across the CNMS, in coordination with our partners in the Neutron Sciences Directorate (NScD), the CNMS User Executive Committee (UEC), and the CNMS Scientific Advisory Committee (SAC), are working diligently to develop near and long-term strategies to address the DOE recommendations. This letter documents our response to the three Action Items and the Recommendation. The development of an updated strategic plan (Action Item 1) and near- to mid-term capability investment strategy (Action Item 2) are underway and a description of the processes being implemented are provided below. A detailed plan with specific milestones and timelines to implement strategic enhancements designed to strengthen the relationship with the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) is provided (Action Item 3), as is a description of efforts being undertaken to enhance outreach efforts and increase our industrial users (Recommendation).

***Action Item 1:** Revisit and update the strategic plan with refined and realigned forward-looking scientific themes that synergistically encompass the full suite of CNMS's capabilities, scientific research activities, and the evolving needs of the user community; ensure continuous*

engagement of the UEC and SAC in defining center-scale strategic priorities and investments. Submit the revised plan to BES by the end of CY 2025.

The CNMS deeply values its dual mission of advancing world-leading science and supporting a dynamic and impactful user program. From its inception, CNMS has emphasized the strong synergy between these two missions. Our in-house thematic research drives the development of cutting-edge capabilities for the user community and serves as a catalyst for attracting leading researchers across a broad spectrum of disciplines. These interactions foster a rich environment of collaboration, where user engagement strengthens and informs our internal science, often guiding the evolution and expansion of our thematic research directions and providing invaluable guidance for future capability investments across the Center.

CNMS has initiated a comprehensive revision of its 5-year Strategic Plan to address Action Item 1, with a strong emphasis on establishing stronger scientific synergy and alignment of its thematic focus areas as well as ensuring that key capabilities are integrated within theme research. This process began with a division-wide listening session held on September 16, 2025, that was led by the Physical Sciences Directorate (PSD) communications team and is being followed-up with targeted surveys to gather input from CNMS staff. This initial session used an established process designed to foster open dialogue and conversation. The CNMS leadership team is committed to transparency; soliciting input from all staff members ensures the creation of a revised Strategic Plan that reflects the best ideas gathered from across the entire division. A primary goal of this initial session was to understand how CNMS staff view the alignment of current theme research efforts with the user program and user needs, allow staff to express how included they feel within the current themes, to gauge how clearly the importance of synergy between the programs has been communicated across the Center, and whether staff feel current practices align with communication on the topic.

CNMS is working diligently to establish a new SAC to assess the effectiveness of both the CNMS science and user programs. The BES operations review was delayed by two years due to the COVID-19 pandemic, which resulted in many SAC members extending their tenure beyond the normal 2-year term. Soon after the operations review in FY24, all the SAC members' terms ended, with many SAC members having served for more than four years. As a result, the CNMS leadership team has identified 10-14 new committee members to invite to serve on the SAC. Our previous SAC engagement model was an experimental approach adopted during the pandemic that was intended to align the scientific expertise of individual SAC members with a specific science theme. Initial conversations with previous SAC members suggested that this approach, which facilitated deeper scientific discussions with our SAC members during monthly Theme Town Halls, was engaging and appreciated by staff and SAC members alike. However, the review panel clearly conveyed that this arrangement was insufficient in garnering the input needed to fully assess the impact and synergy of the combined science and user programs. Thus, we will return to a more standard model of engaging the SAC in both the science and user programs and to this end, we will initiate annual on-site meetings with the SAC starting in early CY 2026 supplemented by regular communications such as weekly Town Halls and monthly calls with the Director. We will also expand SAC representation to include members from

industry, neutron scattering, and the field of artificial intelligence (AI)/machine learning (ML) to garner additional insights to effectively grow our science efforts and user communities in these key areas. The SAC will work closely with CNMS leadership, group leaders, theme leads, and the user program director to provide strategic guidance on building strengths, leveraging opportunities, and establishing strategic directions for the facility. SAC reports will be shared with CNMS staff and ORNL's Associate Laboratory Director for Physical Sciences.

The CNMS restarted Theme Town Halls in February of 2025, which have proven to be extremely valuable for coordinating research and communicating efforts across the Center and are open to all ORNL staff and users working on-site. Each theme lead organizes a Town Hall once each month, with the fourth week reserved for guest speakers. CNMS now broadly advertises the weekly Theme Town Halls and seminars to the CNMS and neutron scattering user communities and the CNMS advisory committees, encouraging their participation, continuous engagement, and to emphasize that we welcome their input regarding scientific directions and future capability development. The CNMS leadership team, particularly the theme leads, are working with staff to coordinate the theme science areas to fully capture the breadth of research and to clarify the extent to which the combined effort of the themes leverages the full suite of capabilities and staff expertise available at the CNMS.

The revised CNMS 5-year Strategic Plan will be submitted to BES by December 31, 2025. This updated plan will be available on the CNMS website and will serve as a living document, with mechanisms established for periodic reassessment and stakeholder engagement to maintain relevance in a rapidly evolving scientific landscape.

Action Item 2: Create a near- to mid-term capability investment strategy that plans for capability retirements, replacements, upgrades, prioritizations, and focuses on optimizing the use of each capability. Submit the plan with its milestones to BES by the end of CY 2025.

CNMS is currently creating a near- to mid-term capability investment strategy that will guide decisions for instrument retirements, replacements, upgrades, and balances the maintenance of current capabilities that are considered foundational with the addition of new cutting-edge instruments and capabilities. This strategy will integrate the scientific needs and impact of major capabilities across both the theme science and user programs. The CNMS leadership team is compiling a list of existing equipment and future investments that clearly articulates the impact and use of each piece of equipment on theme science and the user program, including current working status (age, downtime, etc.), condition of current or future lab space in which it is housed, and the original and current value (cost of service contracts and replacement cost). In addition, we will include estimates of equipment lifetimes. These data will be used to prioritize future investments, taking into consideration immediate needs for the science and user programs, potential vulnerabilities, and the development of unique capabilities.

In addition to equipment investments, the CNMS leadership team is compiling a list of staffing priorities. This working list identifies opportunities (i.e., expanding flow chemistry and

deuterium expertise, growth in AI/ML, alignment with strategic BES/ORNL priorities, etc.) as well as succession planning (i.e., pending retirements), and considers the staffing additions required in terms of research professionals, technical professionals, technicians, and post-doctoral researchers. Our goal is to develop a staffing plan that ensures continued growth and leadership in areas unique to the CNMS and support of critical capabilities needed by our user community.

Maintaining leadership in developing and providing cutting-edge capabilities and theoretical tools is a core priority for the CNMS. We are deepening our investments in AI/ML and autonomous experimentation, advancing the “labs of the future” concept to accelerate discovery for both in-house and user research. Over the next five years, we will continue to craft and refine a capabilities strategy informed by CNMS staff combined with ongoing outreach to the user community. To strengthen engagement with our users, we will work closely with our UEC to explore new and improved ways to collect detailed user feedback. The UEC will pilot follow-on conversations (in addition to the standard BES user surveys) where UEC members will connect one-on-one with CNMS users to gather actionable input on their experiences and identify opportunities for improvement.

Finally, the CNMS is establishing a new electronic instrument reservation and control system that will provide detailed and actionable information about individual instrument utilization across the Center. We are taking a staged approach to install the control system, beginning with instrumentation in the Nanofabrication Research Laboratory and steadily working to incorporate all the major instruments across the CNMS. The data will enable CNMS to limit access to equipment to trained operators, provide information about tool usage by project and user, track instrument down-time, and enable reservations on the individual capabilities.

The final capability strategy will be submitted to BES by the end of CY 2025 and will be incorporated into the CNMS 5-year Strategic Plan.

Action Item 3: *To strengthen the relationship with the SNS and HFIR, provide a plan with specific milestones and timelines to implement strategic enhancements in this area. Submit the plan to BES as part of the 90-day response.*

The CNMS recognizes the critical importance of deepening our strategic and operational connections with the SNS and HFIR. These co-located DOE Office of Science user facilities provide synergistic capabilities that, when more fully integrated, will enable our user community to execute transformative scientific investigations by accessing state of the art complementary infrastructure and working collaboratively with subject matter experts at ORNL. We view this alignment not only as an opportunity to coordinate resources and expertise, but also as a responsibility to the scientific user community to deliver a seamless, synergistic experience for materials discovery, understanding, and translation.

Our plan is a product of discussions with BES program managers and collaborative meetings between CNMS and NScD leadership, scientific staff, and members of the UEC and the SNS-HFIR User Group (SHUG). The proposed initiatives build on existing collaborations in soft matter, theory and modeling, and quantum materials, and recognize the need for integrated AI/ML workflows that harness heterogeneous data. A recent Laboratory Directed Research and Development (LDRD) initiative, Non-Equilibrium and Transients (NEAT), which is sunsetting in FY 2026, has highlighted the power of combining advanced neutron and nanoscale probes, high-performance computing, AI/ML, and new theoretical frameworks to decode the dynamics of non-equilibrium processes across scales in both soft matter and quantum materials. The proposed scientific initiatives described below build on this momentum and outline necessary steps and investments that will continue to optimize strategic alignment.

Our effort to strengthen the alignment between CNMS and SNS/HFIR is focused on three technical and three outreach-oriented initiatives. The three technical initiatives are designed to:

- Define a clear roadmap and investment strategy for establishing a national isotopic substitution capability, encompassing deuteration for neutron studies and isotopic substitution for NMR and related applications such as quantum materials.
- Identify and co-develop complementary characterization and modeling tools that can be coordinated with SNS/HFIR sample environments, creating shared workflows across CNMS and neutron facilities.
- Establish a central theory hub that integrates theory, modeling, and AI/ML workflows to interpret multimodal data streams, maximizing the scientific return from our combined user facilities.

These focused efforts in deuteration and isotopic substitution, co-development of characterization methods and sample environments, and theory-AI/ML integration will be connected through joint research initiatives in areas of high scientific opportunity, including quantum materials, soft matter, and biological interfaces. Together, these efforts will ensure that our shared investments deliver broad impact, strengthen cross-facility interactions, and position our user community at the forefront of scientific discovery.

These technical initiatives will be underpinned by additional investments that focus on cross-facility training, onboarding of users, user outreach, enhancement of cross-facility dialogue through targeted seminars and Town Halls, and shared investment in staff and postdoctoral researcher positions. We aim to further lower the barriers to entry for users working within either facility to more easily access resources across the Centers to ensure that the scientific community can fully leverage the unique strengths of CNMS, SNS, and HFIR. Together, these actions will ensure that our facilities operate not as separate entities, but as an interconnected ecosystem that empowers users to pursue transformative science.

To advance these goals in a tangible and impactful way, the strategic technical initiatives described in detail below will serve as focal points for deepening CNMS–SNS–HFIR integration and enable CNMS to be a gateway for new neutron users. These initiatives span both scientific

investments and operational coordination and are described with proposed milestones and timelines.

Develop a Roadmap for a National Isotopic Labeling Capability

Goal: The goal of this initiative is to define a path and investment strategy for developing a national isotope labeling center dedicated to the chemical synthesis of isotopically labeled materials used in neutron scattering, mass spectrometry, and NMR studies.

Isotopic substitution and deuteration are essential for neutron scattering and NMR since they provide powerful contrast mechanisms, enabling researchers to highlight or effectively mask specific molecular components within complex materials. Establishing a national capability would unlock new insights into structure, dynamics, and function across polymers, biomolecules, and quantum materials, greatly expanding the scientific reach and impact of these techniques.

At present, the U.S. lacks a broad, coordinated infrastructure for the synthesis and characterization of isotopically substituted materials. This limitation constrains the scientific community by narrowing the scope of experiments that can be undertaken by academic researchers, industrial partners, and major national user facilities. Although stable isotopes such as ^2H , ^{13}C , and ^{15}N , provide unique opportunities for advancing our understanding of materials via neutron scattering, they remain underutilized. In developing a roadmap for a national capability, we aim to assess existing resources and user demand for isotopically labeled materials and define the investments needed to build a program that supports this scientific enterprise at scale.

ORNL is well-positioned to lead this effort. CNMS and NScD have decades of shared experience in producing deuterated materials for the user community. CNMS has extensive experience in synthesis of a wide range of isotopically labeled small molecules, monomers, and polymers that have been used in a variety of neutron scattering studies. Recent efforts at CNMS have established a pipeline for the rapid delivery of a select number of deuterated precursors through a rapid-access user proposal mechanism. These offerings are advertised on the CNMS website and provide a valuable entry point for users. Custom deuterated materials can be accessed through the general CNMS proposal system. CNMS has been advancing the development of an autonomous continuous flow reactor synthesis system to scale the deuteration process and broaden the scope of available materials, with automation and ML-guided approaches, offering new opportunities to accelerate production. The Bio-Deuteration Laboratory within DOE's Biological and Environmental Research (BER)-funded Center for Structural Molecular Biology (CSMB) is located at ORNL and is an established specialized hub for the production, purification, and characterization of H/D-labeled biomolecules that are critical for applications ranging from small-angle neutron scattering (SANS) and protein crystallography, to reflectometry and neutron spectroscopy.

CNMS and NScD staff have become deeply integrated in deuteration activities by sharing expertise and cross-training researchers. For example, CNMS staff members regularly engage in cell cultivation, protein purification, and the production of deuterated proteins and bio-derived

molecular precursors using resources in the NScD biology labs. In addition, a CNMS staff member plays a central role in advancing synthesis of deuterated reagents for biological and soft matter neutron scattering studies with support from NScD through the CSMB.

Building on these foundations, our roadmap will outline a staged effort to expand U.S. deuteration capabilities. The initiative will begin with community engagement and benchmarking and will progress toward defining and resourcing a national-scale program. The timeline below outlines the major milestones envisioned for this effort:

Proposed Milestones and Timeline:

- **12 months:** Define community priorities and overall demand by co-sponsoring and hosting a workshop on isotopically labeled materials for neutron scattering and complementary techniques including NMR and mass spectrometry. The workshop will address community priorities for soft and biological molecules, define needed investments in advanced synthesis (including automated and ML-guided approaches), and articulate scientific opportunities and synthesis techniques for isotopes in novel inorganic materials.
- **18 Months:** Complete benchmarking of existing international deuteration resources in Europe and Australia and assess existing isotopic substitution capacity within the U.S.
- **24 months:** Establish an investment framework that articulates investment requirements at multiple operational scales (limited, conservative, aggressive) and begin targeted allocations for laboratory renovations, equipment acquisitions, and staff expansion based on the availability of resources.
- **36 months:** Demonstrate expansion and show tangible progress through completed renovations, staff hires, and the commissioning of new resources. Demonstrate broad user access to expanded capabilities for deuteration and isotopic substitution.

By following this roadmap, the domestic research community will gain access to a sustainable and comprehensive infrastructure to produce isotopically labeled materials. Establishing such a resource will not only greatly strengthen neutron scattering and NMR research, but will also enable breakthroughs in quantum materials, energy technologies, biological systems, and soft matter.

Co-develop Integrated Workflows that Coordinate Emerging Neutron Scattering Sample Environments with Complementary Characterization and Modeling Capabilities at CNMS

Goal: Identify and expand complementary sets of characterization and theoretical tools that can be directly integrated with emerging sample environments at SNS/HFIR, creating workflows that are useful across CNMS and neutron facilities.

This initiative recognizes that CNMS hosts tools and workflows that complement the development of new sample environments and ongoing experiments within NScD, yet these resources remain underutilized. A key reason is the lack of awareness about existing capabilities, points of contact, and mechanisms for access. Beyond simply improving communication, this initiative will create intentional, augmented tools and workflows that explicitly link CNMS and neutron scattering capabilities, ensuring connections are not only clear, but also purposefully designed, integrated, and optimized to maximize impact.

We envision the creation of seamless, end-to-end workflows that integrate sample environments at SNS/HFIR with the advanced characterization and modeling capabilities at CNMS. By linking sample preparation, nanoscale characterization, and modeling with neutron experiments, this effort aims to maximize the efficiency and impact of beamline science. The outcome will be accelerated discovery through coordinated experiments, automated quality control and workflow scheduling, integration of high-throughput methods with computational modeling, and the ability to focus neutron beamtime on the most unique and high-value experimental conditions identified through AI/ML insights.

To realize this vision, we will invest in complementary instrumentation and shared platforms that extend the reach of both facilities. CNMS tools will be strategically developed to augment neutron scattering environments, as demonstrated by recent joint investments in the Superconducting Quantum Interference Device (SQUID) magnetometer, which expanded magnetic characterization capabilities relevant to beamline users. Other future examples include deploying and augmenting dynamic and static light scattering capabilities to complement SANS sample environments and upgrading broadband dielectric spectroscopy (BDS) equipment at the CNMS into the RF regime to align with neutron spin-echo and quasi-elastic neutron scattering (QENS) timescales. A more extensive table showing possible neutron experiments, existing complementary capabilities, and potential future investments is provided in Appendix A. A working group consisting of staff from the NScD sample environment groups and CNMS staff with a deep familiarity with NScD beamline capabilities will identify and prioritize opportunities for shared resources such as robotic liquid handling, ellipsometry, and prescreening pipelines that ensure sample quality, stability, and homogeneity prior to neutron experiments.

A cornerstone of this effort is the integration of data and modeling across the two facilities. Centralized pipelines will be developed to standardize and unify experimental data into searchable, long-term databases accessible to users. These resources will be coupled with a CNMS-hosted Theory, Modeling, and AI/ML Hub that connects experimental workflows with advanced simulations, including density functional theory (DFT) and molecular dynamics (MD), as well as physics-based predictive models (see below). Such integration will enable dynamic model development and AI-driven predictions of material structure, dynamics, and functionality under diverse conditions. In doing so, the combined CNMS–NScD ecosystem will provide users with a powerful platform for data-rich, predictive, and highly coordinated materials research.

Proposed Milestones and Timeline:

- **12 months:** Establish a working group and survey current capabilities and emerging sample environments to identify opportunities for co-developed toolsets and identify co-funded workflow teams.
- **18 months:** Prototype and validate three integrated workflows/sample environments and pilot availability within the SNS/HFIR proposal system.
- **24 months:** Track adoption, gather user feedback, and target **15+ user projects** leveraging shared workflows.
- **36 months:** Demonstrate integration of experimental workflows with the Theory, Modeling, and AI/ML Hub pipeline.

Establish a Central Theory and AI/ML Hub to Integrate Theory, Modeling, and AI/ML Workflows for Multimodal Data Interpretation

Goal: Build a CNMS–NScD Central Theory and AI/ML Hub that integrates theory, modeling, and AI/ML workflows with cross-facility experiments, enabling efficient interpretation of complex multimodal datasets and delivering transformative insights into materials behavior.

Nanoscience and neutron scattering probe materials at vastly different length and time scales. Theory, modeling, and AI/ML provide the essential computational framework to integrate these perspectives, enabling connections that yield deeper insight into material behavior. The Hub will enable researchers to decode quantum phenomena, unravel the dynamics of soft and biological matter, and design next-generation data workflows that accelerate insight far beyond what neutron scattering, nanoscale experiments, or modeling alone can achieve. This synergy will not only enhance the precision, interpretability, and predictive power of experiments, but will also create new paradigms for materials design, discovery, and control. This investment in shared computational frameworks, user-facing tools, and cross-divisional expertise will amplify the reach and impact of both CNMS and SNS/HFIR. Ultimately, the Hub’s scientific impact lies in accelerating the discovery cycle itself, turning complex data into actionable knowledge, reducing the path from hypothesis to result

The Hub will serve as a CNMS–NScD cross-divisional platform for advancing theory, simulation, data workflows, and AI/ML with a science focus that spans quantum materials, soft-matter and biophysics, and data-driven workflows integrated with ML, aligning directly with CNMS science themes. These domains represent areas where predictive modeling and computational discovery are tightly coupled to experimental advances and where high-performance computing (HPC) platforms can accelerate scientific impact. By embedding this Hub within CNMS and SNS/HFIR and leveraging ORNL’s computational and experimental strengths, the initiative will enable transformative insights into fundamental materials behavior while creating a robust foundation for future BES priorities.

The Hub will directly connect CNMS and NScD through showcase projects designed to bridge simulation, data, and experiment. Projects will be solicited from staff and users across both facilities, prioritized through a steering committee that will be CNMS–NScD-led, with participation from other ORNL divisions. The SACs of CNMS and NScD will play a role in guiding the steering committee’s activities. These projects will enrich CNMS science themes while catering to the needs of neutron scattering experiments, creating a bidirectional integration where theory, computation, and experiment jointly shape research directions and accelerate discovery. Outreach will include a joint seminar series with broad lab-wide participation, along with visible highlights that demonstrate cross-facility integration to DOE and the broader community. In addition, user-facing cloud-based tools, open software, and branded communication platforms (e.g., a Hub webpage) will make the Hub’s capabilities broadly accessible.

Sustaining the Hub's success requires dedicated personnel investments. Long-term plans include establishing staff positions embedded within the CNMS's Theory and Computation Section, specifically the Nanomaterials Theory Institute (NTI) and Data NanoAnalytics (DNA) groups, that will be jointly funded by CNMS and NScD and will support the growth of computational tools and cross-facility workflows. These staff will serve as bridges between divisions, enabling continuity in high-impact projects and ensuring that innovations developed in the Hub are maintained and expanded. Early career staff and postdocs will play a central role through hands-on involvement in seed and showcase projects, fostering professional development while strengthening the Hub's intellectual base. This investment will secure the Hub's long-term vitality, enabling it to attract a broad joint user base and maintain leadership in simulation–experiment synergy.

Proposed Milestones and Timeline:

- **12 months:** Establish the CNMS–NScD Theory and AI/ML Hub steering committee (with SAC participation) and identify 3–5 high-impact cross-facility science cases where theory, computation, and experiment can be tightly integrated.
- **18 months:** Launch two pilot showcase projects that demonstrate bidirectional integration of simulations, ML-enabled data workflows, and SNS/HFIR experimental measurements, with early deliverables (e.g., prototype pipelines, shared datasets).
- **24 months:** Deploy a shared computational framework, including cloud-based data storage, open-source tools, and workflow automation, to support reproducible theory–experiment integration across CNMS science themes and neutron scattering experiments.
- **36 months:** Scale the Hub to support at least 10 active user projects annually, with participation spanning multiple CNMS science themes and SNS beamlines and establish a joint seminar series highlighting results and methods.

Success of the Hub will be measured by the demonstrated scientific impact of high-profile joint publications, open software releases, or community tools, showcasing the Hub as a national model for theory–experiment integration at BES user facilities.

While these strategic science initiatives define the future directions of our joint research and facility investments, their ultimate value depends on how effectively they are communicated to, and leveraged by, the user community. Scientific advances in isotopic substitution, integrated experimental pipelines, or Theory, modeling, and AI/ML-enabled workflows will only achieve their full impact if users are aware of the opportunities, can access the resources seamlessly, and feel supported in building collaborations that span CNMS, SNS, and HFIR. In this sense, outreach, education, and proposal development efforts are not secondary activities but essential components of our strategy, ensuring that the science we envision translates into real user engagement and productivity.

To that end, we are prioritizing new mechanisms that strengthen the connections between users and facilities, fosters collaboration across modalities, and equips researchers with the tools they need to maximize scientific return. Initiatives such as joint seminar and proposal planning series, coordinated proposal review and user-matching systems, and expanded cross-facility training and onboarding programs are designed to lower barriers to participation, build shared scientific

culture, and drive co-developed proposals. By investing in these “softer” but equally critical elements of engagement, we will ensure that our strategic science initiatives are visible, accessible, and impactful, thereby enabling CNMS, SNS, and HFIR to deliver on their mission as national scientific resources. These efforts are listed below with a brief description of goals, milestones, and timeline for the proposed activities.

Expand Cross-Facility User Training and Onboarding Programs

Goal: Better educate users and staff on how to effectively leverage multimodal resources across CNMS, SNS, and HFIR.

To achieve this goal and bring together the user communities we will work with NScD to co-develop webinars and in-person workshops starting with Neutrons 101, an introduction to neutron scattering, and encouraging CNMS staff and users to participate in the Neutron Scattering School held annually at ORNL.

Proposed Milestones & Timeline:

- **12 Months:** Co-develop and deliver Neutrons 101, a 3-module training series for new users to introduce them to neutron scattering.
- **18 Months:** Launch a CNMS–SNS–HFIR User Roadmap and Handbook, an online resource to guide users through the process of utilizing multiple facilities through a single proposal submitted to either CNMS or Neutron Sciences.
- **24 Months:** Strive to have at least 100 users participate in the Neutron 101 series annually.
- **36 Months:** A 25% increase in cross-facility usage by trained users will be the initial goal of these efforts.

Launch Joint Virtual Seminar and Proposal Planning Series

Goal: Deepen connections with the user community by holding regular, co-hosted events that build thematic collaborations and proposals involving CNMS and NScD.

CNMS currently holds weekly Town Halls to discuss, review, and refine our theme science directions. Going forward, we will invite SNS/HFIR staff to participate in the Theme Town Halls. The first step will be to identify points of contacts within NScD that align with each of the CNMS themes and encourage them to share weekly agendas and discussion topics with other relevant NScD staff. We anticipate this will lead to more collaborative research between the two user facilities and an increase in joint user proposals from the CNMS and NScD user communities.

Proposed Milestones & Timeline:

- **12 Months:** Co-host six joint virtual seminars and two proposal planning workshops with neutron sciences.
- **18 Months:** Track and increase attendance at the seminars and workshops by 20% annually over the next two years and solicit feedback to refine topics of interest.
- **24 Months:** Receive at least 10 jointly developed user proposals from seminar and workshop attendees.

- **36 Months:** Launch an annual joint proposal call for CNMS and NScD users, built around a unifying theme such as Quantum Across Modalities.

Implement Joint Proposal Reviews and a User Matching System

Goal: Expeditionously screen user proposals that would benefit from utilizing both CNMS and neutron scattering capabilities through the utilization of AI/ML resources.

Once identified, staff will reach out to the principal investigator for further discussion. Ultimately, this tool will be incorporated into the online proposal process to allow users to self-screen their proposals for complementary capabilities.

Proposed Milestones and Timeline:

- **12 Months:** Benchmark proposal co-screening tool using existing FY 2026 user proposals and verify the accuracy of the results on at least 100 proposals.
- **18 Months:** Launch beta AI/ML tool to suggest integrated facility access for FY 2027 user proposals and follow up with principal investigators of the selected proposals.
- **24 Months:** Embed AI/ML tool into the CNMS online proposal system workflow with a target of identifying 10% of user proposals for potential cross-facility opportunities.
- **36 Months:** Monitor conversion and refine tool to achieve a new target to identify 20% of user proposals submitted through the tool.

The combined set of strategic technical initiatives and user-focused outreach efforts outlined here represent a cohesive framework for strengthening the integration of CNMS with SNS and HFIR. These actions will not only expand our scientific capabilities but will also ensure improved visibility and facility accessibility and will be impactful for the user community. To demonstrate accountability and value, we have articulated clear milestones and will track progress through measurable outcomes such as joint proposals, user engagement metrics, and cross-facility utilization, and report these regularly to DOE and to our user communities. In doing so, we will create a transparent process that highlights successes, identifies areas for continuous improvement, and ensures that our collective efforts remain aligned with national scientific priorities. Ultimately, this coordinated strategy will position CNMS, SNS, and HFIR as a truly integrated ecosystem that delivers transformative science.

Recommendation 1: CNMS should continue to strengthen its outreach efforts to increase industrial users

CNMS recognizes the importance of expanding industrial engagement and remains committed to strengthening outreach efforts to attract a broader spectrum of industry users. We have initiated discussions with the other NSRCs to identify routes toward revising user agreements to streamline industry access and provide fluid access across the Centers. ORNL leadership is working with our partnership and legal offices to seek mechanisms for implementing further improvements.

We will expand industry representation on our SAC and UEC and convene a panel of experienced industrial users to identify challenges, opportunities, and value propositions. Their

insights will guide both near- and long-term strategies to enhance industrial access and collaboration. Additionally, we will continue to expand and highlight collaborative partnerships with industries that enable the development of new ‘first of their kind’ capabilities that can be showcased to the user community. These efforts will be integrated into our broader strategic and capability planning processes, ensuring that industrial user engagement and partnerships continue to grow as an integral component of CNMS’s mission going forward.

Past initiatives have included revising the CNMS proposal research description section to invite technical developments and achievements along with fundamental science questions, increasing the number of industrial representatives on the proposal review committee, and creating a dedicated seat for industry on the CNMS UEC.

In addition to the steps described above, expanded efforts to increase the number of industrial users are outlined below. This plan positions CNMS to attract more industry users and partnerships while also accelerating translation of fundamental material discoveries into solutions for industrial stakeholders. By deepening collaborations, participating in national forums, showcasing impact, investing in staff education, and advancing intellectual property development, CNMS will strive to broaden its industrial user base, accelerate co-developed technologies, and demonstrate a broader impact on U.S. innovation.

Leverage ORNL’s Industrial Partnerships and Economic Development Group

ORNL’s partnerships office has a team of outreach specialists whose efforts are focused on industry outreach and identifying capabilities at ORNL that may be valuable for potential industrial partners. We identified the need to more effectively communicate what the CNMS can do for potential partners and understand barriers to connecting CNMS capabilities with industry needs. CNMS will actively coordinate with ORNL’s Industrial Partnerships and Economic Development groups to:

- **Leverage established networks** to identify potential industrial collaborators.
- **Align partnership models** (e.g., CRADAs, SPPs, licensing) with CNMS strengths in nanomaterials synthesis, characterization, theory, computation, and development of autonomous experiments.
- **Engage closely with the ORNL Partnerships Office and PSD communications teams** to increase visibility to both local and national businesses by producing accessible and meaningful content that effectively communicates CNMS capabilities in a manner that highlights potential impact for industrial users.
- **Streamline engagement** by providing clear points of contact and coordinated messaging between CNMS and ORNL’s Partnerships Office.

Active Participation in Industry-Focused Conferences and Symposia

CNMS staff actively present at national and international scientific conferences. However, we will work with our partnerships office and industry advisory committee members to identify additional opportunities to connect with industrial stakeholders by:

- **Presenting and exhibiting at national meetings** (e.g., MRS, AVS, ACS, battery and semiconductor industry meetings) that draw strong industrial participation.

- **Organizing symposia and workshops** that highlight CNMS capabilities and user success stories directly relevant to industry needs.
- **Expanding general outreach and education** at professional meetings and community engagements, positioning CNMS as both a research and education hub.

Capture and Highlight Industry Impact using Additional Metrics

Capturing only numbers of industry users provides limited data as to the level of engagement and impact that the CNMS has with respect to industrial partnerships. Working with the industry members of our UEC and SAC, we will work to define additional metrics that provide a richer account of industry engagement and impact, such as:

- **Track and recognize in-kind investments** such as co-development of capabilities, methodologies, and computational workflows.
- **Highlight existing partnerships** through case studies, communications, and reporting to demonstrate CNMS's broader impact on industry innovation.
- **Share success stories** that showcase how industrial collaborations translate into economic value, intellectual property, and technology adoption.

Provide Education and Staff Development for Industry Engagement

CNMS recognizes the importance of equipping staff to navigate industry collaborations. Often the legal and logistical hurdles of establishing industrial partnerships can be daunting for staff and users. To lower the perceived barriers and facilitate staff engagement with industrial users we will:

- **Provide education opportunities** for staff to understand licensing pathways, intellectual property management, and partnership mechanisms.
- **Hold training workshops** to enhance staff understanding of the commercialization process and DOE/ORNL partnership structures.
- **Empower researchers** to translate their scientific advances into industry-relevant outcomes.

Increase Intellectual Property, Innovation, and Technology Development

CNMS will align its innovation strategy with industry and DOE priorities by:

- **Increasing the number of patents and invention disclosures** emerging from CNMS research.
- **Encouraging alignment with a long-term vision** of building CNMS-driven equipment, software, and integrated research tools from scratch.
- **Developing joint IP strategies** with industrial partners that create mutual value while preserving the open science mission of the user facility.

Proposed Milestones and Timeline:

- **12 Months:** Familiarize ORNL's Partnership and Economic Development Group with the capabilities and research at CNMS and create a one-page handout tailored to industrial users, attend local networking events identified by ORNL's Partnership and Economic Development Group, host a technology transfer seminar for CNMS staff, and attend industry specific conferences.

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- **18 Months:** Develop methodology and metrics to capture and report in-kind investments from industrial partners.
- **24 Months:** Increase CNMS and CNMS-partnered patents and invention disclosures output by 20% compared to FY 2024.
- **36 Months:** Increase the number of industrial proposals submitted by 30% compared to number in FY 2024.

This formal 90-day response is intended to update DOE with our progress on addressing Action Items 1 and 2 and to fully address Action Item 3 and the Recommendation provided by DOE-BES to improve operations at the CNMS. This response will be followed with our updated 5-year Strategic Plan and capabilities investment strategy that will be submitted to DOE-BES by the end of CY 2025.

CNMS and ORNL leadership would like to thank BES and the panel of reviewers for their time and thoughtfulness in providing the CNMS with a comprehensive and detailed review of theme science and user programs. We are pleased with the overall positive outcome of the review.

Sincerely,



Scott T. Retterer

Director

Center for Nanophase Materials Sciences

cc: Linda Horton, SC
Cynthia Jenks, ORNL
Dava Keavney, BES/SUF
Harriet Kung, SC
Rocio Meneses, BES/SUF
Karren More, ORNL
Bindu Nair, BES
Andy Schwartz, BES/SUF

Appendix A – Table of Complementary Instrumentation and Potential Investments

Neutron Experiments	CNMS capabilities	Potential CNMS Investments
Small-angle neutron scattering (SANS)	• Multi-angle static/dynamic light scattering • Electrophoretic mobility/zeta potential measurements • Nano differential scanning calorimetry (DSC) • MD simulations • Lorentz transmission electron microscopy (TEM) and 4D-STEM • Magnetic properties measurement system (MPMS) (1.8 K to 1000 K)	
Rheo-SANS	• Rheo-small-angle-light-scattering • Rheo-optical-microscopy • Nonequilibrium MD simulations	
SANS/liquid reflectometry with humidity cells	• Small-angle X-ray scattering (SAXS) • Ellipsometry	• Humidity cells (~\$15K) • Humidity generator (~\$80K)
SANS/Broadband dielectric spectroscopy	• Broadband dielectric spectroscopy	
SANS w/ dynamic light scattering (DLS) or static light scattering (SLS)	• Multi-angle static/dynamic light scattering • molecular dynamics simulation • MPMS (optical option)	
Photoelectrochemical liquid reflectometry	• Quartz crystal microbalance with dissipation monitoring (QCM-D) • Ellipsometry	• Ellipsometry upgrade (~\$300K)
Regular liquid reflectometry	• QCM-D • Ellipsometry • MD Simulations	• 4-QCM-D liquid handling systems (~\$120K)
Rheo-liquid-reflectometry	• Nonequilibrium MD simulations	
Polarized neutron reflectometry (PNR)	• MPMS • Ferromagnetic resonance (FMR) insert for physical property measurement system (PPMS) • Lorentz TEM and 4D-STEM • Spin-polarized scanning tunnelling microscopy (STM) • Scanning nitrogen vacancy (NV) microscope	• Magneto optic Kerr effect (MOKE) microscope 0.5T vector magnet and low temperature stage (~\$250k) • Cold stage insert with 1T magnet compatible with cathodoluminescence scanning electron microscope (CL-SEM)

		and existing optical systems (~\$250k)
Dynamic electronic or optically pumped reflectometry	• PPMS 9T 1.8K-400K • Probe stations - room temperature	• PPMS 14T with rotation stage and multifunction platform (\$700k) • Broadband electronic and RF gating sources (~\$175k)
Neutron spin-echo and QENS	• Broadband dielectric spectroscopy • MD simulations	• Impedance analyzer (~\$200K) • Network analyzer (~\$270K)
SNAP pressure beamline	• MPMS high pressure cell	