

Advancing U.S. Leadership: The Science Case for a Second Target Station at the Spallation Neutron Source

Report on the Scientific Grand Challenges and Renewed Vision for the Second Target Station

March 2026



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**ADVANCING U.S. LEADERSHIP: THE SCIENCE CASE FOR THE
SECOND TARGET STATION AT THE SPALLATION NEUTRON
SOURCE**

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March 2026

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ABBREVIATIONS

AI	artificial intelligence
AM	additive manufacturing
BEI	Bragg-edge imaging
BES	DOE Office of Science Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
CSNS	China Spallation Neutron Source
DOE	U.S. Department of Energy
ESS	European Spallation Source
FTS	First Target Station
HFIR	High Flux Isotope Reactor
INS	inelastic neutron scattering
ML	machine learning
NIST	National Institute of Standards and Technology
NScD	ORNL Neutron Sciences Directorate
nGI	neutron grating interferometry
ORNL	Oak Ridge National Laboratory
QFI	quantum Fisher information
QS	quorum sensing
QSL	quantum spin liquids
SANS	small-angle neutron scattering
SEI	solid–electrolyte interphase
SNS	Spallation Neutron Source
STS	Second Target Station
STS-DGS	STS direct geometry neutron chopper spectrometer
STS-IMG	neutron imaging instrument at STS
STS-LR	liquids reflectometer at STS
STS-SANS	small-angle neutron scattering instrument at STS
STS-SCD	STS single-crystal diffractometer
TOF	time of flight

EXECUTIVE SUMMARY

The United States faces urgent scientific and technological grand challenges that exceed the capabilities of current neutron sources and other available characterization tools. The Second Target Station (STS) is a transformative scientific facility designed to address grand challenge science and achieve U.S. scientific and technological leadership. For centuries, advances in technology have been closely tied to advances in the tools of science. The U.S. Department of Energy (DOE) national laboratories provide the foundation for U.S. innovation, housing a one-of-a-kind collection of powerful research user facilities. Among them, DOE Office of Science Basic Energy Sciences (BES) user facilities, including light and neutron sources, have played a central role in scientific breakthroughs, energy innovations, and national security. These facilities have underpinned major advances, contributing to some of the 118 Nobel Prizes associated with the DOE.

Neutron scattering is a core capability in the complex of DOE user facilities. Neutron sources and X-ray sources are essential complementary tools used by science to advance critical discovery and understanding for technological breakthroughs. Often, these facilities are the decisive tools behind important innovations. Neutrons are generally considered more penetrating than X-rays and are incredibly sensitive to magnetism, light elements (such as hydrogen and lithium), and isotopes. These capabilities enable classes of experiments that are not possible with X-rays. Neutrons provide unparalleled insights into the structure, dynamics, and behavior of novel materials and scientific phenomena, including those used in quantum technologies, manufacturing, and nuclear technology.

Recognizing the strategic importance of neutron scattering, the Basic Energy Sciences Advisory Committee (BESAC) in 2024 emphasized the importance of advancing STS at Oak Ridge National Laboratory (ORNL). BESAC recognized that STS has “the potential to be absolutely central to future world-leading science,” and recommended building a compelling science case to support STS as a priority for maintaining U.S. scientific leadership.

ORNL took this opportunity to engage the national community to refine the STS science case and convened a national workshop held August 23–26, 2024, in Washington, D.C., chaired by leading scientists—Alan Tennant (ORNL, University of Tennessee, Knoxville), Soichi Wakatsuki (Stanford University), Norman Wagner (University of Delaware), and Laura H. Greene (Florida State University, National High Magnetic Field Laboratory)—to identify the key scientific opportunities uniquely enabled by STS. A detailed list of participants is provided in Appendix A.

The workshop brought together 104 experts from national laboratories and leading universities to define the grand scientific challenges that must be addressed to maintain U.S. scientific leadership and the characteristics and capabilities STS must have to enable transformative scientific discoveries in those essential areas. The workshop committee ultimately identified 10 specific grand challenges around the following 5 science themes, which are described below and in Table ES1.

Quantum Materials: STS will propel a quantum-enabled future by providing experimental ground truth for discovering and validating quantum materials and enabling the study of entanglement, decoherence, and quantum interactions in ways no other method can. It will probe quantum states at the nanoscale, enabling for the first time neutron spectroscopic investigations of thin films of 10 nm and above. STS will enable Hamiltonian validation that can be used to directly verify quantum computing results and reveal hidden quantum phases under extreme conditions, unlocking the potential for next-generation quantum technologies and accelerating the transition from materials to devices, ensuring U.S. leadership in the quantum race.

Engineering and Manufacturing: STS will revolutionize the understanding of materials performance under real-world, in-use conditions—from atomic-scale defect formation to large-scale mechanical behavior. STS will provide transformative capabilities for additive manufacturing and construction that will reduce costs and provide the United States with advantages in accelerating next-generation manufacturing technologies.

Chemistry and Catalysis: STS will transform chemical research by revealing the atomic and molecular mechanisms governing catalysis, energy, and critical U.S. industrial applications. It will provide real-time insights into catalytic transformations, which are critical for energy security and supply-chain resilience.

Soft Matter: STS will provide real-time visualization of the dynamics and structure of polymers and soft materials, combining atomistic and mesoscale resolutions. This enhanced understanding of the self-assembly of polymers will enable transformative development of designer materials for consumer products and the energy sector.

Biology: STS will unlock new understanding in biomolecular interactions, self-assembly, biological adaptability, biomolecular condensates, and disease-related protein dynamics, driving advancements in drug development, personalized medicine, and antimicrobial applications, including bio-preparedness.

This document describes research areas the community considers to be the highest priority grand challenge research directions that will deliver the highest scientific impact by leveraging the unique capabilities of the STS source. For each science theme, two grand challenge priorities have been chosen as exemplar cases for which STS will provide unique experimental insights. Community experts consider these challenges to require the unique information that neutron scattering provides over what is possible at current light sources. Furthermore, investigating these areas is not possible with current neutron facilities available to U.S. researchers.

Table ES1. Ten grand challenges aligned with STS capabilities.

Theme	Grand challenge	STS relevance
Quantum Materials	Grand Challenge 1: Discover Quantum materials that approach fundamental limits for information and energy technologies	STS will accelerate discovery of quantum materials and understanding of quantum states, enabling advancements in quantum computing, spintronics, and quantum sensing.
	Grand Challenge 2: Advance understanding of quantum coherence and fundamental dynamics in materials platforms	STS will provide unique understanding of entanglement and decoherence through entanglement witness measurements of quantum states.
Materials Science and Engineering	Grand Challenge 3: Accurate digital twins to accelerate discovery and development of new materials	STS will provide real-time, high-resolution data on materials under extreme conditions, confirming predictive models and accelerating certification.
	Grand Challenge 4: Materials and processes for autonomous construction innovation	STS will enable unique in situ imaging and real-time measurements of strain, solidification, and deformation—essential for additive manufacturing and robotics-based construction.

Table ES1. Ten grand challenges aligned with STS capabilities (continued).

Theme	Grand Challenge	STS Relevance
Chemistry and Catalysis	Grand Challenge 5: Unlocking the fundamental mechanisms governing catalysis	STS will visualize catalytic reactions in realistic environments, revealing reaction mechanisms critical for energy and chemical production.
	Grand Challenge 6: Advancing chemical science for a resilient energy future	By probing reaction pathways and molecular transformations, STS will enable developments of advanced fuels, separation technologies, and energy systems.
Soft Matter and Polymers	Grand Challenge 7: Understanding dynamics in nonequilibrium systems	STS will capture molecular motions and mesoscale reorganization during flow, curing, or ion transport—essential for energy and manufacturing materials.
	Grand Challenge 8: Mastering hierarchical assembly and multiscale design	STS will provide simultaneous multiscale observation of assembly processes, revealing how structure and chemistry determine material function, unlocking the full potential of additive manufacturing.
Biological Systems	Grand Challenge 9: Engineering the principles of life	STS will enable neutron protein crystallography on small samples, unlocking structure and hydrogen bonding data for key enzymes and drug targets.
	Grand Challenge 10: Understanding the molecular basis of health, aging, and well-being	STS will reveal biomolecular interactions, conformational changes, and proton dynamics critical to disease mechanisms, bioenergy, and synthetic biology.

Realizing the STS Vision Through Strategic Investment and Integration

STS is designed to provide a transformative leap in neutron capabilities, offering researchers access to the highest peak brightness cold neutrons in the world. Its innovative U.S.-developed source design, instrumentation, and data infrastructure will open new frontiers in materials characterization and time-resolved studies. STS is not an isolated project—it is the cornerstone of a broader, integrated vision for neutron science at ORNL.

The vision for STS has been carefully developed, with key milestones reflecting a long-term national commitment to advancing neutron science. From early conceptual studies and workshops (1996–2015) through design refinements and strategic planning, the project has steadily matured. Between 2016 and 2019, ORNL finalized major design choices and launched the Proton Power Upgrade project as a critical step to upgrade the accelerator system toward STS operation. From 2020 to 2023, the project advanced through critical DOE approvals, facility design planning, and early infrastructure work. In 2024, the Proton Power Upgrade achieved 1.7 MW proton beam on target, confirming the accelerator’s readiness for STS. With the evolution and developments in science and innovation, the BESAC report served as the trigger to refresh the science cases and ensure that STS simultaneously addresses the most pressing scientific questions and closes a critical characterization gap in the U.S. facility portfolio. In 2025, DOE approved Critical Decision-3A to initiate site preparation earthworks—a significant step toward construction.

Current U.S. Neutron Source Landscape

The United States currently operates three open-access user neutron sources, two located at ORNL as DOE user facilities—the High Flux Isotope Reactor (HFIR) and the First Target Station (FTS) at the

Spallation Neutron Source (SNS)—and one located at the National Institute of Science and Technology Center for Neutron Research, which has been in an unplanned maintenance shutdown since 2021. These facilities support a wide range of scientific research but cannot, on their own, meet the growing demand for advanced neutron capabilities across the national scientific enterprise. Ensuring continued U.S. leadership in materials research, quantum science, energy dominance technologies, and advanced manufacturing requires strategic investment in infrastructure that keeps pace with emerging scientific needs and competing nations.

The 3-Source Strategy at Oak Ridge National Laboratory

The 3-Source Strategy (Figure ES-1) is a forward-looking plan to secure U.S. leadership in neutron science by leveraging the complementary strengths of three co-located neutron sources at ORNL: HFIR, FTS, and STS. Each source is designed to optimize a different aspect of neutron generation and use, creating a comprehensive and unmatched neutron science ecosystem. HFIR is a high-flux continuous reactor that provides an exceptionally high time-averaged flux of neutrons, making it ideal for experiments requiring a continuous flux of neutrons with moderate wavelength resolution. FTS, a pulsed spallation source, produces high-intensity thermal neutrons (and some cold neutrons) with the highest achievable temporal resolution, making it ideal for studies that require fast, time-resolved data on the structural dynamics of materials.

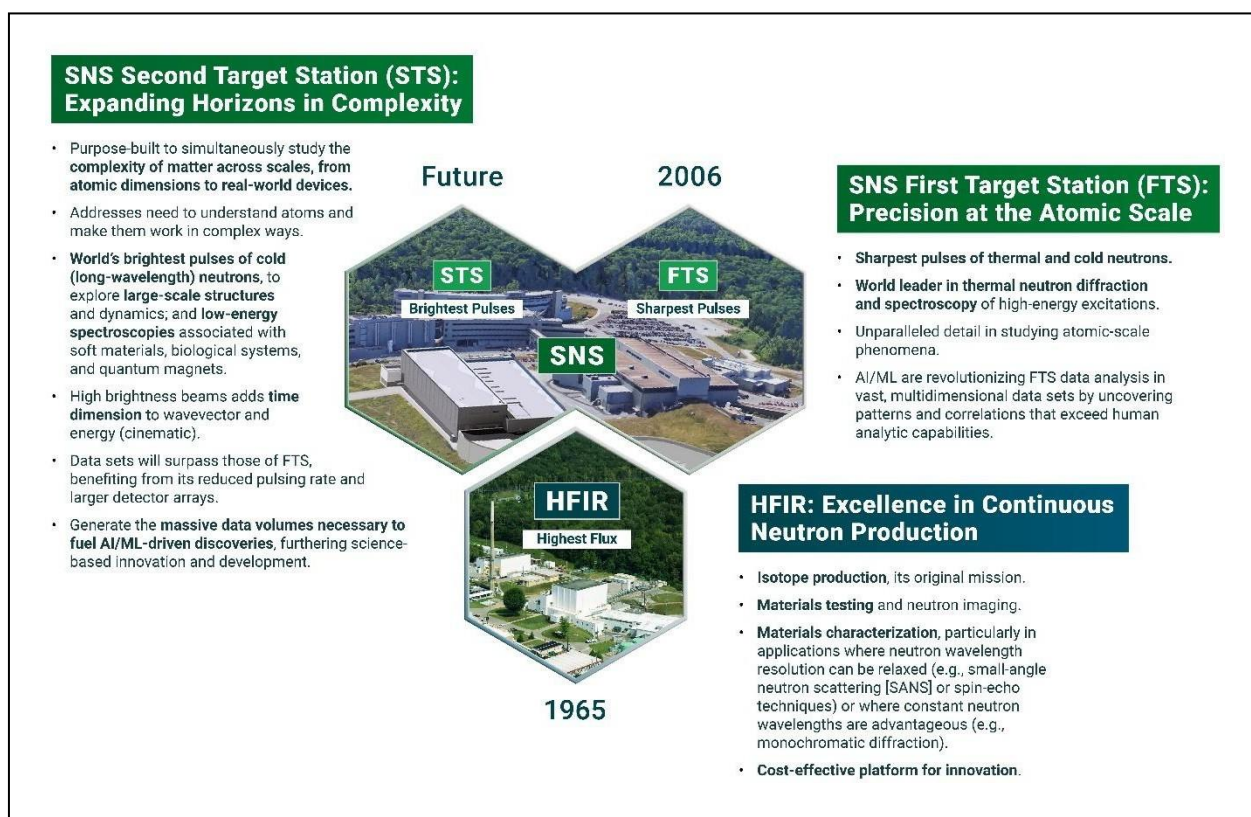


Figure ES-1. ORNL 3-Source Strategy. Image courtesy of ORNL.

STS, the third pillar of the strategy, will extend U.S. science capabilities by providing the world's highest brightness of pulsed cold neutrons. STS will enable high-fidelity studies of atomic, nanoscale, and mesoscale structures, allowing transformative studies in quantum materials, chemistry, engineering, soft

matter, and biology. It will fill a critical gap in U.S. capabilities and provide access to a suite of experiments that are currently not possible at any neutron facility.

These three sources are not stand-alone facilities but components of an integrated neutron ecosystem at ORNL. Together, they offer researchers flexibility, efficiency, and the ability to pursue cross-cutting experiments that benefit from multiple neutron capabilities. The strategy maximizes return on prior investments in SNS and HFIR. For example, ORNL has completed the Proton Power Upgrade, which doubled accelerator beam power and provides the necessary capacity to feed FTS and STS. This project is already delivering science, positioning ORNL to move forward with STS construction without delay. The 3-Source Strategy ensures that each facility supports and extends the capabilities of the others, creating a nationally coordinated resource for materials discovery and technological advancement and sharing common resources and infrastructures.

Transformational Capabilities at the Second Target Station

STS will be optimized for high peak brightness cold neutron production, operating at 15 Hz with a compact moderator system designed to deliver broad neutron bandwidth in a single measurement. The optimized para-hydrogen moderators and rotating tungsten target are engineered to produce intense, short-pulse cold neutrons. STS achieves significantly higher peak brightness than currently possible globally, allowing for transformative experimental modalities that include multimodal investigations and, critically, the ability to measure sub-milligram sample quantities (Figure ES-2).

STS will produce neutron beams with 10 times the brightness of FTS, surpassing current capabilities in Europe and China. The neutron source enables construction of neutron scattering instruments with unparalleled scientific capability that will open new avenues of research and lead to transformative scientific discoveries. Researchers will be able to observe dynamic processes in real time, gaining insight into fast-moving reactions and phenomena that were previously out of reach,

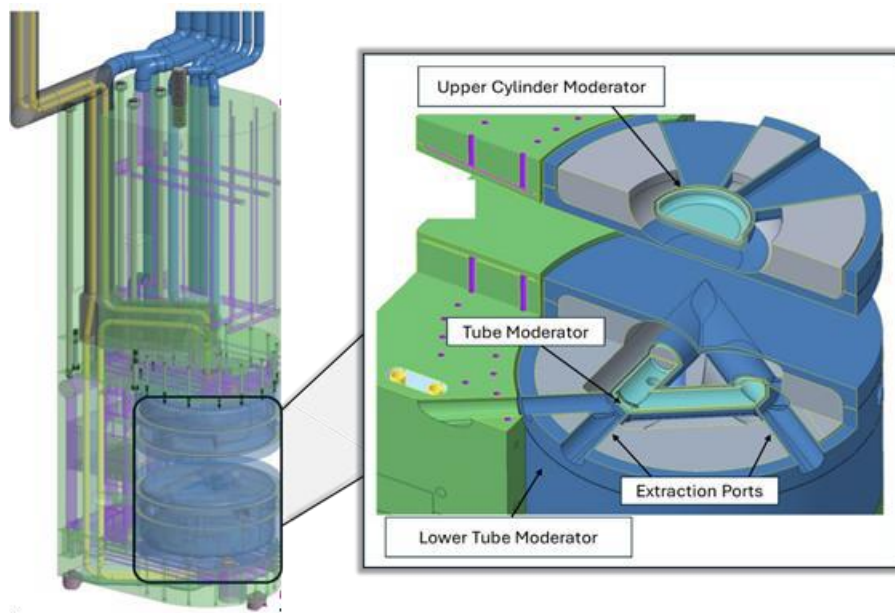


Figure ES-2. Detail view of STS moderator. Image courtesy of STS.

with the ability to collect usable data per pulse. STS advances are particularly significant for studying quantum platforms and magnetism, where the unique sensitivity of neutrons to magnetic properties will allow researchers to probe the fundamental interactions in magnetic materials and devices with unprecedented clarity. Key capabilities include microelectronvolt-resolution spectroscopy with a broad dynamic range for probing quantum materials and energy landscapes as well as pump-probe experiments with 10 ns resolution to capture real-time responses to external stimuli across interfaces and devices.

Single-pulse data collection will accelerate experimentation in reflectometry, diffraction, and spectroscopy, while multimodal setups will enable simultaneous measurement of structural and dynamic properties. As illustrated by specific examples in subsequent sections, the combined STS capabilities will yield individual instruments gains of over 100 times the current state-of-the-art instrumentation available today. As an overall scientific capability, STS will provide high-fidelity datasets with thousands of times more detail than is currently achievable, producing a data lake of high-quality science data for artificial intelligence (AI) that can be used to develop accurate science foundation models that will be used to further accelerate discovery. Researchers will be able to study much smaller samples—essential for nanomaterials, thin-film devices and quantum platforms, and biomolecular systems—and monitor time-dependent changes as they happen. These advances will significantly accelerate discovery in key scientific and technological areas, from understanding the quantum behavior of new materials to developing next-generation manufacturing processes.

Enabling U.S. Leadership in Priority Research Areas

STS is positioned to drive advances across a range of high-priority scientific and technological domains. In quantum science, STS will provide the magnetic sensitivity, spatial resolution, and energy needed to detect quantum states, coherence, and entanglement across material interfaces. This level of detail is essential for validating and improving the performance of quantum devices, which are highly sensitive to material defects and instabilities, allowing the technology to move from materials to devices and prototypes. In advanced manufacturing, STS will make it possible to monitor phase transitions and structural evolution during additive processes such as 3D printing. STS will enable 3D tomographic strain mapping with micrometer precision, supporting advanced material design and providing critical insights into the mechanical properties of materials at multiple scales critical for advancing manufacturing and construction material.

Researchers will be able to record high-fidelity, time-resolved sequences of complex phase transitions, capturing experimental data on out-of-equilibrium transient phenomena or metastable phases. Combined with FTS characterization tools and AI-powered analytics, STS will support materials-by-design strategies that accelerate the delivery of novel products to market.

In the energy sector, STS will allow researchers to observe radiation-induced changes in nuclear materials under realistic conditions. This capability supports the development of digital twins—computational models of reactor components that use real-world data to predict performance and failure. These tools will reduce costs, accelerate license processes, and improve safety for fusion and fission systems, driving the advancements of U.S. energy infrastructure.

A National Investment in Scientific Infrastructure

STS is not a routine facility enhancement. It is a major national investment in the tools and infrastructure required to support U.S. scientific leadership for decades to come, unleashing its full potential in quantum materials, chemistry, engineering, soft matter, and biology and maintaining competitive leadership over other nations. It addresses urgent gaps in domestic capabilities and provides researchers with access to critical experimental techniques.

Global competitors are rapidly expanding their neutron science capabilities. Without STS, the United States risks falling behind in fields critical to economic competitiveness, national defense, and energy dominance. Accelerating the construction of STS will contain project costs, deliver key capabilities sooner, and support the development of emerging industries tied to quantum technologies, energy, biomedical devices, and advanced manufacturing.

STS is the third pillar of ORNL's 3-Source Strategy and a complementary component of the nation's basic science ecosystem, with facilities that drive technological breakthroughs critical for energy, engineering, and innovation while closing a critical characterization gap. The community continues to be extremely supportive and enthusiastic about the potential for STS to address the most pressing science and technological grand challenges (Table ES1). Accelerating the construction of STS is imperative for enabling technological breakthroughs in emerging areas important to U.S. industry. Moreover, an accelerated project timeline will lead to significant cost savings. Most importantly, the longer the delay, the further the U.S. will fall behind competing nations, potentially suffering irreversible technology gaps in fields such as quantum science.

1. INTRODUCTION

The U.S. Department of Energy (DOE) Office of Basic Energy Sciences (BES) suite of world-leading research infrastructures ensures the critical scientific priority of maintaining U.S. leadership in materials and life sciences. Construction of the Second Target Station (STS) at ORNL is a critical next step in maintaining that leadership by expanding U.S. neutron science capabilities into measurement regimes not accessible at existing facilities. Neutron scattering is an essential tool for advancing materials research across many disciplines, offering unique insights that cannot be obtained by other methods while supporting the national economy and addressing critical challenges in quantum materials, chemistry, engineering, soft matter, and biology. STS is a major scientific capability advancement, combining high-brightness moderators, advanced neutron transport optics, innovative neutron scattering techniques and detectors, and cutting-edge integration of artificial intelligence (AI) and computational advances, while fully leveraging the completed proton power upgrades to the SNS accelerator complex. STS is central for the U.S. research community to maintain global scientific leadership in a period that sees stronger than ever competition from China and Europe.

In May 2024, the Basic Energy Sciences Advisory Committee evaluated future construction projects proposed by the DOE Office of Basic Energy Sciences, including STS (Anderson et al., 2024). The committee recognized that STS has “the potential to be absolutely central to future world-leading science” but recommended that “the science case must be more fully developed to specify the currently inaccessible grand challenges that the new capabilities can address.”

The ORNL Neutron Sciences Directorate (NScD) initiated an activity in June 2024 to engage the community and revisit the original STS science case (Adams et al., 2019). NScD leadership formed a committee that included Professors Alan Tennant (University of Tennessee, Knoxville), Laura Greene (Florida State University, National High Magnetic Field Laboratory), Norman Wagner (University of Delaware), and Soichi Wakatsuki (Stanford University). During workshops and meetings that extended through July 2025, the committee worked closely with the national scientific community to redefine the science case and vision for STS (Appendix A). The workshop included input from seasoned as well as early-career scientists across various fields that benefit from neutron scattering as well as researchers who use complementary techniques such as synchrotron X-rays and free-electron lasers. Together, the workshop participants evaluated the unique capabilities of neutrons and STS, identifying scientific challenges that only STS can address. This report highlights the community-defined transformational science essential for maintaining U.S. leadership and outlines how STS is designed to meet these needs. This report also describes the performance of the source and the expected capabilities of a reference instrument suite showcasing the scientific potential of STS, aligning with the scientific community’s need to sustain U.S. leadership in science and technology. A complementary community-driven report will also be developed and will include additional scientific challenges to which STS can contribute. Community engagement will continue as part of the STS project, ensuring that STS capabilities meet the needs of emerging high-priority science themes.

STS is a transformative leap in neutron science, providing access to well-separated neutron pulses at the required energy or wavelength with the intensity and spectral sharpness (brilliance) needed to fill the current discovery and characterization gap in U.S. and global facilities. With these capabilities, STS will drive breakthroughs in critical science and technology areas, enabling progress from “pixel power” to “voxel power.” This evolution allows for six-dimensional exploration of material properties through spatial, temporal, momentum, and energy resolutions. STS offers unmatched capabilities and is crucial for addressing major scientific challenges, unlocking breakthroughs in quantum materials, advancing the development of materials into devices, and enhancing manufacturing and biomaterials, all while enabling U.S. energy dominance. A key takeaway from this process is that the United States is at a critical point in neutron science. The U.S. science and technology community urgently needs to close the existing

characterization gap and provide access to world-leading scientific infrastructure that can address pressing issues. These issues require the ability to access long length scales and systems out of equilibrium. U.S. scientists need neutron capabilities that provide very bright beams of cold neutrons and allow fast, low-latency experiments to study out-of-equilibrium phenomena and excitations. Additionally, the U.S. neutron beamline capacity is far below requirements, slowing scientific progress and hindering U.S. international competitiveness and, in turn, economic development (Walsh et al., 2024). STS will deliver the necessary beamlines and groundbreaking capabilities in a cost-effective and timely manner.

The scientific case for STS has evolved significantly over the past decade, reflecting shifts in scientific priorities, the growing influence of AI, and the increasing urgency of national challenges that neutrons from STS are uniquely positioned to address. Box 1.1 presents the various phases of the STS project, beginning with initial ideas in the late 1990s and culminating in significant progress achieved today.

Box 1.1: Timeline of the Second Target Station

The timeline outlines key milestones in the development of the Second Target Station (STS) project at Oak Ridge National Laboratory (ORNL), tracing its roots from early conceptual studies in the late 1990s to major project advancements in 2024. This progression highlights ORNL's long-term commitment to advancing neutron research capabilities, with STS positioned as a future cornerstone of scientific innovation.

1996–2015: Initial studies and workshops recommended an upgraded accelerator and additional target sources at the Spallation Neutron Source to ensure future U.S. scientific leadership. STS Critical Decision (CD)-0 was awarded in 2009. A series of “grand challenge” workshops shaped the project’s science goals, addressing emerging research needs.

2016–2019: ORNL refined the STS science case and technical design. Major design decisions, including a 700 kW proton beam and 15 Hz pulse rate, were confirmed, and the project office was established. The Proton Power Upgrade was launched, providing additional power to the First Target Station and the capacity to prepare the accelerator for STS.

2019: ORNL published a first experiments report, describing examples of first experiments to be conducted at STS in five key science areas: polymers and soft materials, quantum matter, materials synthesis and energy materials, structural materials, and biology and life sciences.

2020–2021: Key project approvals, including CD-1 by DOE, allowed for preliminary designs and instrument selection. Architecture and engineering contracts were awarded for STS facility designs.

2022–2023: Construction on essential infrastructure, such as a stub tunnel for future STS connection, progressed alongside expert advisory board reviews to ensure project success.

2024: Beam commissioning for the Proton Power Upgrade reached 1.7 MW on target, a significant milestone demonstrating the accelerator’s future capability for STS needs. The Basic Energy Sciences Advisory Committee acknowledged STS’s central role in global scientific advancement, recommending further development of its scientific goals. That recommendation led to national engagement with the science community and two reports: a community report and this report.

2025: DOE granted CD-3A approval to support site preparation for construction, including preliminary earthworks and rough grading of the construction area.

2. SECOND TARGET STATION IS ESSENTIAL FOR U.S. SCIENCE

The DOE national facility portfolio is impressive, especially its world-leading neutron and light source facilities. These facilities are essential for materials characterization and fuel innovation: they provide deep insight into the structure of materials at an atomic level, including atomic locations, dynamic behavior, and resulting functionalities. Neutron and light sources work together to advance discovery and the deployment of many important innovations.

However, a gap currently exists in the characterization spectrum provided by these national facilities, one that the STS facility will close. STS will offer new insights that are currently inaccessible with existing capabilities, enabling transformative research across a range of scientific areas. By providing higher brightness and bandwidth, STS will open new windows into the complex behavior of matter across multiple length scales. STS will enable experiments on microgram samples, breaking through size barriers that have previously limited the use of neutrons, for example, to measure excitations in thin films. The broad bandwidth combined with focusing optics and high solid-angle detector coverages will produce the massive, high-fidelity datasets needed to fuel AI/machine learning (ML)-driven discovery. The intense STS neutron beams will allow researchers to study materials in action—as they are made, as they evolve, and as they fail—in some cases with single pulses of the source.

Neutron scattering and synchrotron X-ray scattering are complementary analytical techniques, each with distinct advantages for materials science. Neutrons interact with materials via nuclear forces and magnetic dipoles; the neutron scattering cross section is not proportional to atomic number, making neutron scattering equally sensitive to light atoms as well as heavy elements, magnetic structures, and isotopic differences, providing good contrast between elements with similar atomic numbers. X-rays interact electromagnetically with electrons, offering high spatial resolution and good sensitivity to heavier elements.

X-ray techniques allow for fast, high-resolution measurements; however, the interaction between photons and the sample can result in ionization damage and sample heating effects. Neutron scattering does not induce radiation damage by ionization or sample heating effects, making the technique especially useful for studies of quantum effects, for delicate soft matter and biology science, and for studies of structure and dynamics at ultralow temperatures in the 1mK to 4 K region. Neutron scattering is the gold standard probe of magnetic structure in materials.

In recent years, advances at ORNL's First Target Station (FTS) have begun to change the paradigm for neutron scattering, enabling experiments with much smaller samples. STS will take these improvements even further, and its unprecedented neutron brightness will allow for faster data collection and improved sensitivity. This capability will enable experiments that require not only smaller samples but also higher resolution and precision, particularly in fields such as quantum materials, biology, energy, and chemistry.

These advancements, including the development of next-generation microelectronics, energy systems, and advanced polymer composites for structural applications, will significantly accelerate research in critical fields. The insights gained from STS will provide essential scientific understanding that will eventually realize high technology readiness level devices for quantum computing, sensing, and networking, supporting the continued growth and innovation of materials used in these applications. Historically, neutron facilities have had a profound influence on fields such as superconductivity, semiconductors, and aerospace engineering, and STS will continue this trend by enabling new research in areas ranging from energy systems to innovative materials for consumer technologies. Currently, the National Institute of Standards and Technology (NIST) research reactor is not operational, leaving only two open user neutron sources in the United States: the High Flux Isotope Reactor (HFIR) and the SNS FTS at ORNL. STS is being developed as part of ORNL's 3-Source Strategy (Figure ES-1) to

complement these existing sources. Whereas FTS focuses on thermal neutrons with sharp temporal resolution for high-precision atomic measurements, HFIR is optimized for isotope production and specialized neutron scattering techniques. STS will focus on high-brilliance cold neutrons for small samples, dynamic systems, and high-resolution data-driven studies across a broad range of length and time scales, making it an indispensable tool for complex and evolving research needs.

In this new era, where AI and computing technologies accelerate progress, STS will enable breakthroughs by providing high-quality data that can fuel emerging technologies. AI tools will be applied to gain deeper insights into hierarchical systems, offering new opportunities to master the physical world and unlock the benefits of this accelerated progress. The integration of AI and ML with neutron scattering will empower researchers to analyze complex data more efficiently and uncover patterns that were previously inaccessible, opening new avenues for scientific discovery and technological advancement.

2.1 GLOBAL COMPETITION IN NEUTRON SCIENCE IS SET TO ECLIPSE THE UNITED STATES

The capabilities provided by FTS established the United States as an international leader in neutron science. However, the global landscape for neutron sources has shifted significantly over the last two decades, with major international investments challenging U.S. leadership in this field. Europe, Asia, and Australia are advancing their capabilities, while the United States faces challenges related to aging infrastructure and impending capability gaps. This global competition in neutron science underscores the urgency for the United States to modernize its neutron research infrastructure.

Investments in STS and, in the longer term, the Pressure Vessel Replacement project at HFIR, are critical to maintaining U.S. leadership, supporting emerging scientific needs, and enabling world-class research. Without such investments, the United States risks falling behind Europe, China, and Japan in delivering next-generation neutron capabilities essential for advancing science and technology, as illustrated in Figure 1.

2.1.1 European Growth

Europe has made remarkable progress in neutron science, solidifying its commitment to being competitive in global research endeavors. ESS exemplifies this ambition, with an investment exceeding \$3 billion, establishing it as a next-generation mega facility. ESS is designed for high neutron flux and brilliance, offering insights into material structures and properties. Initially operating at 2 MW with 15 instruments by the early 2030s, the facility has a clear upgrade path to operate at 5 MW. Although it surpasses the current cold neutron (5 Å) capabilities of U.S. facilities such as FTS, its peak brightness would still fall short of STS.

Despite the high operating power of ESS (up to 5 MW), the longer pulse duration limits its brilliance compared with STS. By contrast, STS, with its 0.7 MW power and neutron pulses that are 1/20 as long, delivers significantly higher brilliance, enabling unique experiments, including single-shot capabilities. Leveraging advancements in neutron production technology, STS will significantly surpass the capabilities of ESS's long-pulse design, fully capitalizing on the existing accelerator and infrastructure at ORNL. STS will ensure U.S. leadership for decades to come—if STS is realized with an aggressive timeline.

The United Kingdom's ISIS Neutron and Muon Source also reflects Europe's excellence in neutron science. Its low-frequency 10 Hz Target Station 2 has demonstrated highly efficient neutron production at under 100 kW, with two neutron scattering target stations sharing a single accelerator. Looking ahead, ISIS plans to develop ISIS-II by the 2030s, featuring a 1.6 MW high-resolution target (30 Hz) and a

0.8 MW cold neutron target (15 Hz) facility. Complementing these efforts are France’s Institute Laue-Langevin and Germany’s Forschungsreaktor München II, both of which continue to provide high-brilliance neutron beams from reactor facilities and world-class research opportunities.

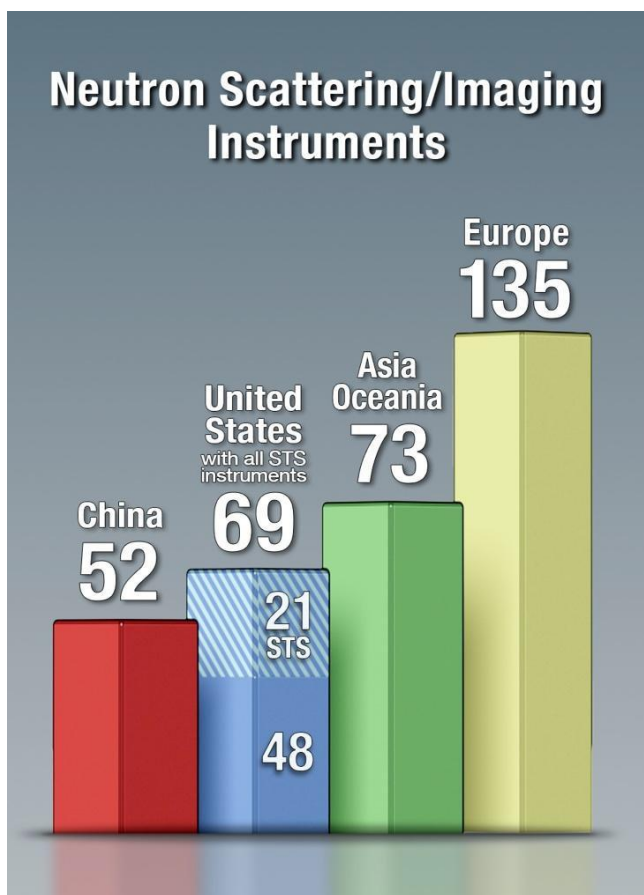


Figure 1. Number of neutron scattering/imaging instruments by region. Europe leads with 5 facilities and 135 instruments, followed by Asia–Oceania (excluding China) with 4 facilities and 73 instruments. China operates 3 facilities with 52 instruments, and the United States has three facilities (HFIR, SNS-FTS, and the currently shut down NIST Center for Neutron Research reactor) with 48 instruments. A fully instrumented STS would contribute an additional 21 instruments, bringing the U.S. total to 69. *Image courtesy of Duncan Harryman/ORNL.*

2.1.2 Asia–Oceania Growth

Asia has rapidly expanded its neutron science capabilities, driven by significant investments and a push for technological independence (Figure 2). China has established itself as a key player, with three new neutron facilities built in the past decade, including the China Spallation Neutron Source (CSNS), which was inaugurated in 2018 (first neutrons in 2017). CSNS currently operates at 160 kW, with 11 instruments, and is upgrading to a 500 kW proton beam by October 2029, with 21 instruments and a muon source. This upgrade will bring CSNS to parity with FTS in the scientifically crucial cold neutron range. Once complete, the CSNS facility will have 21 beamlines, compared with the current 19 beamlines at FTS. In addition, China operates the 60 MW China Advanced Research Reactor, with 18 beamlines and instruments, and the 20 MW China Mianyang Research Reactor.

Using the latest instrumentation and advanced design philosophy, China could surpass the United States in neutron research for the first time in history. China has prioritized its neutron capabilities, recognizing

them as essential to its future scientific and technological ambitions. Japan has also made substantial advancements with its 1 MW Japan Proton Accelerator Research Complex Materials and Life Science Experimental Facility. This mature facility operates with 23 neutron and 4 muon instruments, and it plans to expand with a second target station at 0.5 MW, operating at 7.2 Hz, to improve its capabilities with a design concept similar to that of STS. Japan’s broader neutron science ecosystem also includes the Japan Research Reactor-3, the Kyoto University Research Reactor Institute, and the Neutron Science Laboratory Institute for Solid State Physics at the University of Tokyo, each supporting specialized research programs.

The 30 MW Korean High-Flux Advanced Neutron Application Reactor restarted in 2024 after a prolonged shutdown and is now accelerating its capability development. The Australian government operates the 20 MW Open-Pool Australian Light-Water Reactor for both scattering and isotope production.

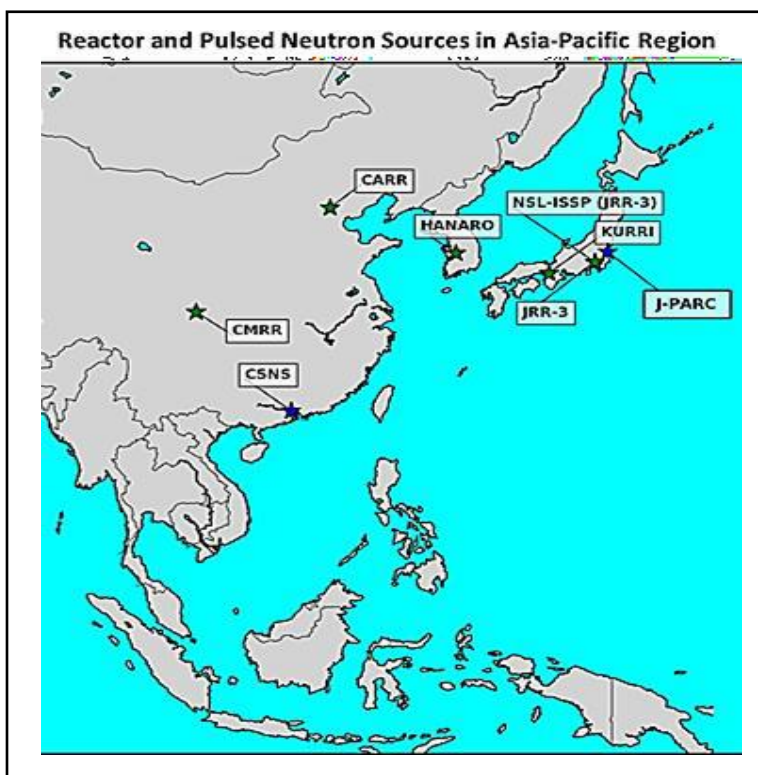


Figure 2. Map highlighting key research reactors and spallation facilities in Asia. Green stars indicate reactor-based neutron sources; blue stars represent pulsed (spallation) neutron sources. *Image courtesy of Theresa Ahearn/ORNL.*

2.2 ELEMENTS CONTRIBUTING TO STS WORLD-LEADING PERFORMANCE

STS represents a major advancement in neutron scattering capabilities. It will provide experimental capabilities that are unmatched by current neutron sources, enable investigations that can be successfully completed only at STS, address critical scientific questions that cannot be solved with existing facilities, and close the characterization gap in the U.S. facility portfolio. The technical specifications of STS are driven by the nation’s science and technology needs, with a focus on stringent requirements that no other facility can meet. Mapping these scientific needs to the required neutron capabilities enables high temporal and spatial resolution, high cold-neutron flux, and broad neutron bandwidth. Together, these features provide the dynamic range needed for complete Q coverage in structural and spectroscopic

measurements within a single pulse. The combination of improvements and STS capabilities described in the following paragraphs results in individual instrument gain factors of at least 100 over the current work leading neutron scattering instrumentation.

These specifications will be achieved using U.S.-developed target and moderator designs and ORNL accelerator technologies. STS will deliver cold (5 \AA) neutrons in 15 Hz pulses, reaching the highest brilliance with fully separated neutron pulses across broad wavelength spectra. As shown in Figure 3, many elements contribute to the world-leading performance of STS.

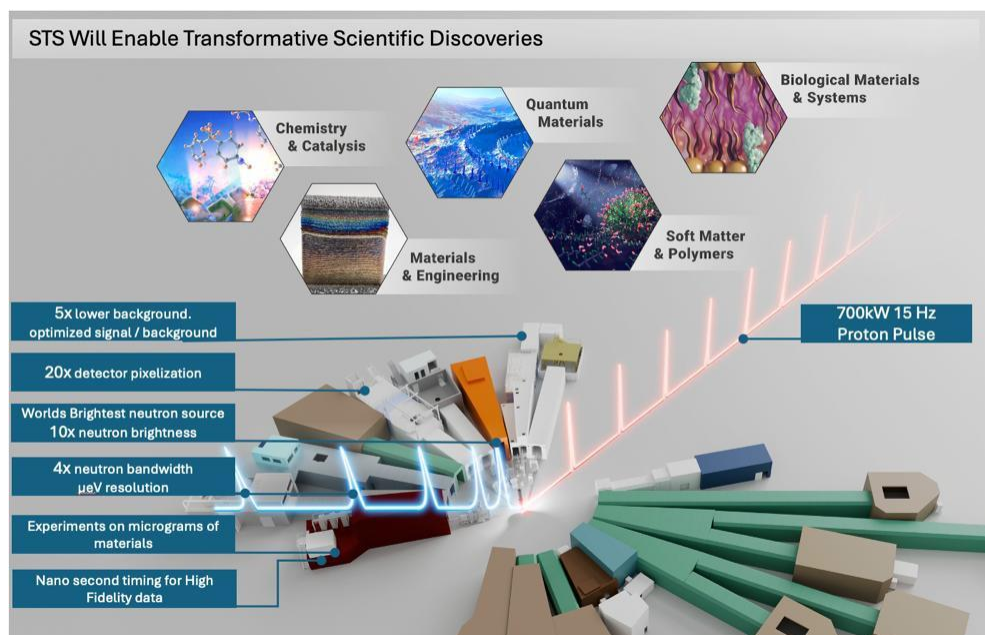


Figure 3. STS key parameters and capabilities for neutron scattering. Listed gain factors are relative comparisons with capabilities at FTS. *Image courtesy of Phoenix Pleasant/ORNL.*

2.2.1 Neutron Source

For many years, sample volume has been a limiting factor for neutron scattering. This limitation is being addressed by the development of high-brightness, low-dimensional moderators, as shown in Figure 4. The figure illustrates the target, reflector, and beamport arrangement, along with the high-brightness cylindrical and triangular para-hydrogen moderators coupled with a water pre-moderator.

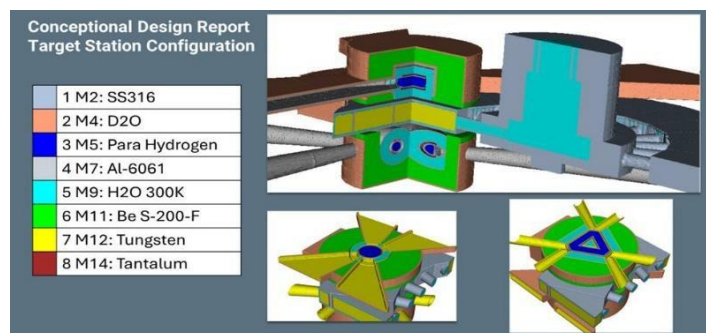


Figure 4. STS target reflector and moderator configuration. Detail views highlight the (lower left) coupled cylindrical and (lower right) triangular para-hydrogen tube moderators. The target reflector and moderator use a water pre-moderator, designed to improve neutron neutronic efficiency. The diameter of the tube moderators is 30 mm. Yellow denotes ports for neutron instruments. *Image courtesy of ORNL.*

The heart of STS is its neutron source moderators and target. The optimized cold neutron moderators at STS will be 10× brighter than those at FTS, and the cold neutron brilliance at STS will be a world-leading 5× more intense than the pulses produced by the 2 MW ESS. The facility will operate at a 15 Hz duty cycle, optimized for 4× broader neutron wavelength bandwidth than FTS. The wavelength bandwidth and brightness of the neutron source have been optimized to offer the highest gains achievable for neutron scattering and provide the world’s most capable neutron scattering facility. The optimized source enables design of the most advanced neutron instruments with capabilities that are not available at existing neutron facilities. The 15 Hz repetition rate is not just an operational feature; it underpins new classes of time-resolved, high-resolution neutron scattering experiments, enabling six-dimensional material insights that define STS’s mission and value. To illustrate the innovative engineering behind this breakthrough, Figure 5 details the proton beam flow and the specialized roles of the target stations.

STS is specifically optimized to generate high-brilliance neutron pulses operating in the cold wavelength regime where neutron optics are most effective. It will deliver the most intense pulses of cold neutrons, representing a critical step forward in the nation’s cold neutron capabilities (Figure 6).

Access to high-intensity, short-pulse cold neutrons at STS is now possible because of recent and ongoing developments in spallation targets; new concepts for high-brightness, low-dimensional, compact, geometrically optimized moderators; advances in neutron transport and focusing; and accelerator technologies that achieve high-availability operation of high-charge-density, short proton pulses. Key drivers of these advancements include cutting-edge target and moderator technologies (Figure 7). Major instrument components such as neutron polarizers and transport optics become more efficient at longer neutron wavelengths, enabling highly effective and precise neutron delivery to instruments.

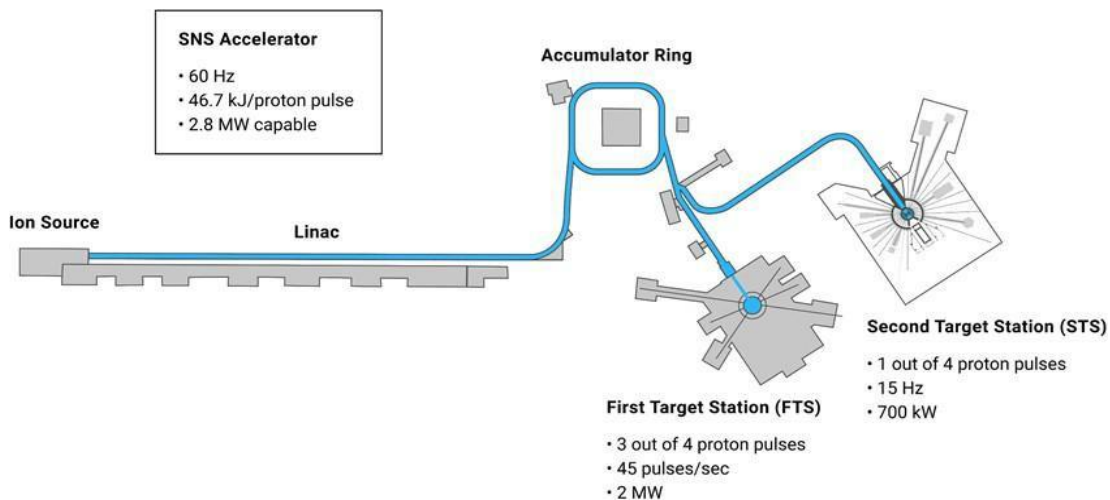


Figure 5. Simplified schematic of SNS. Shown is the proton beam flow from the ion source through the linac, into the accumulator ring, and distribution to FTS and STS. FTS receives three out of every four proton pulses (45 pulses per second at 2 MW), and STS receives one out of every four pulses (15 pulses per second at 700 kW). The 15 Hz operation will be enabled by the upgraded SNS accelerator, which delivers 60 proton pulses per second at full intensity. STS will receive one out of every four of these pulses, operating at 700 kW while FTS continues uninterrupted at its full 2 MW. Each SNS pulse delivers 46.7 kJ of energy in less than 1 μs, producing sharply defined bursts of neutrons that support high-precision time-of-flight measurements. Combined with a high-density rotating tungsten target and compact moderator geometry, this setup produces extremely bright cold neutron emissions. *Image refurbished with enhanced resolution and color by Phoenix Pleasant/ORNL.*

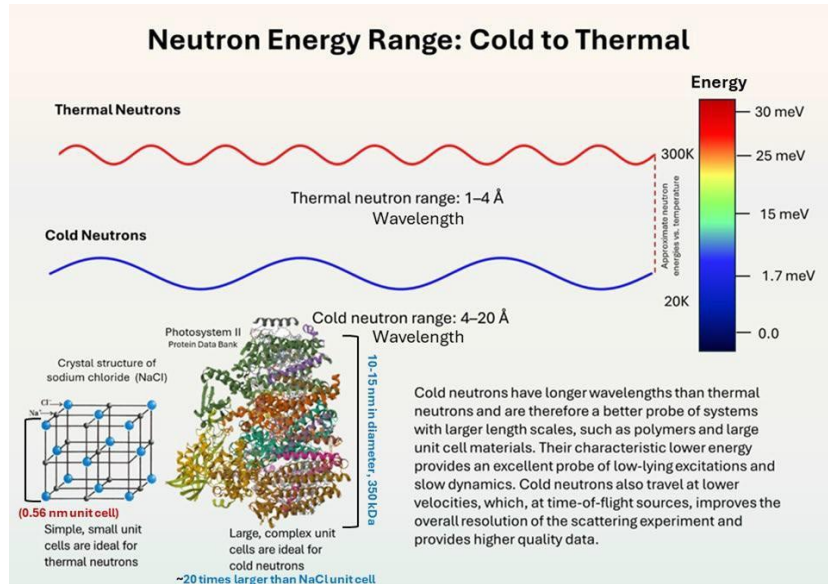


Figure 6. Neutron energy range, from cold to thermal. STS cold neutrons, with wavelengths in the range of 3.5–20 Å, are essential for addressing today’s most pressing challenges in quantum materials, chemistry, engineering, soft matter, and biology. *Image Courtesy of Theresa Ahearn/ORNL.*

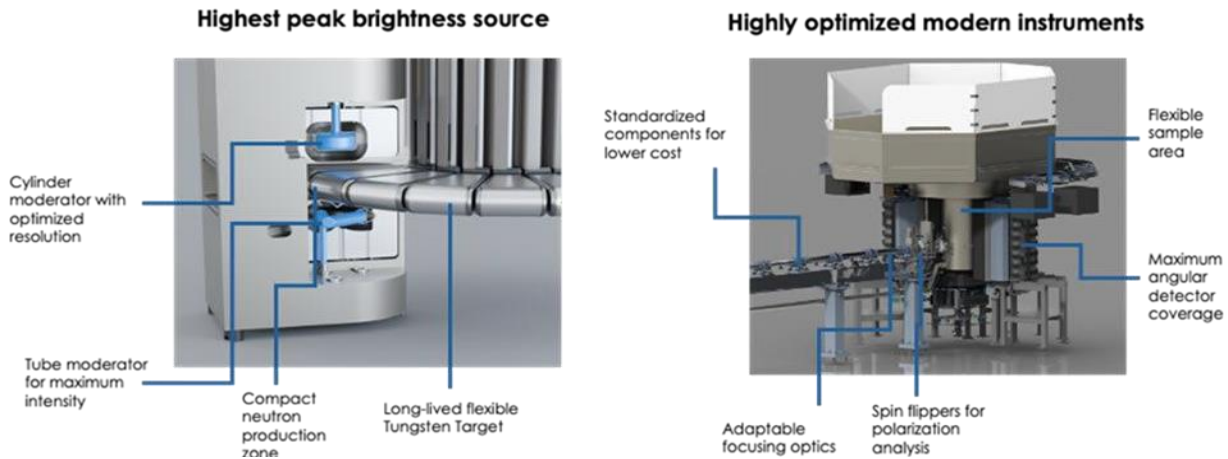


Figure 7. The STS source (left) and instrument performance gains (right). *Image courtesy of STS/ORNL.*

2.2.2 Next-Generation Neutron Instruments

STS enables design of next-generation multimodal neutron instruments that are optimized to efficiently utilize the high source brightness and broad bandwidth and allow per-pulse neutron scattering measurements at 15Hz, enabling a new paradigm of operando, time-resolved neutron science. The STS neutron instrument suite will be developed in close collaboration with the U.S. neutron scattering community, and the instrument road map will be chosen via a clear and transparent selection process that will consider capabilities at FTS, HFIR, and other U.S. neutron facilities within the context of a U.S. roadmap for neutron science. A draft timeline of this process is presented in Section 9 of this document.

Single-pulse measurements: The high source brightness allows single-pulse measurements for all neutron scattering techniques.

Repetition rate multiplication: The large bandwidth at STS will allow simultaneous measurements using neutrons of multiple individual wavelengths in a single pulse. Unlike monochromatic measurements that use only one neutron wavelength per pulse, repetition rate multiplication will enable significantly more data to be collected at once, making spectroscopy experiments more efficient and allowing simultaneous probing of a broad dynamic range of excitations.

Samples: High-brightness moderators at STS will enable focused neutron beams, allowing routine experiments on microgram-sized samples. Smaller samples volumes are typically available earlier in the research cycle, so this capability will improve efficiency and accessibility for cutting-edge investigations and support high-throughput studies of dynamics and structure and game-changing transformation of the materials design lifecycle.

Unprecedented time resolution: The high brilliance will support experiments with time resolutions as fine as 10 ns, compared to 10 μ s at FTS. By bridging the gap between neutron spectroscopy and time-resolved measurements, STS will enable groundbreaking studies of ultrafast phenomena and kinetics in materials.

High-fidelity data: High neutron brightness coupled with state-of-the-art instrumentation and detectors will allow STS to produce datasets that have far greater data fidelity than is currently available. Data acquisition with nanosecond resolution (compared with today's state-of-the-art microsecond resolution) from detector systems that have up to 20 \times greater pixel density will produce rich datasets that capture structural dynamical information in far greater detail, allowing advances in scientific computing like AI and super-resolution methods to be leveraged to extract data features that could be missed with today's facilities.

Instrument sensitivity: The STS repetition rate and overall facility construction have been specified to produce low neutron background signals.

Multimodal instrument design: Instruments designed to simultaneously measure diffraction, small-angle neutron scattering (SANS), and spectroscopic signals will offer comprehensive characterization of complex materials. This capability will help scientists better understand how structure, dynamics, and function are interconnected across multiple scales, enabling research in materials science, biology, chemistry, and engineering that is not currently feasible. These advances will open entirely new areas of study that cannot be addressed with existing sources. STS will accelerate progress by providing unprecedented access to brighter, pulsed neutron beams paired with state-of-the-art instruments optimized for studying materials in real time under realistic conditions.

Spectroscopy and dynamics of thin films and heterostructures at millikelvin temperatures: For the first time, researchers will be able to use inelastic neutron scattering (INS) to investigate spin dynamics in 10 nm thin films, layers, and engineered heterostructures to obtain direct measurement of the dynamic scattering function $S(Q,\omega)$ with high resolution. This capability—often described as a “killer application”—will be essential for uncovering the effects on entangled states, coherence, and exotic quasiparticles as system size and dimensionality are reduced from bulk materials to lower dimensions. Theoretical predictions of emergent and unusual phases of matter at interfaces will require experimental validation, and STS is uniquely positioned to enable such investigations.

Ultrafast time-resolved measurements with 10 ns pump–probe capabilities: STS will allow researchers to study transient, out-of-equilibrium processes. This capability is essential for understanding dynamical behaviors predicted to be essential for many areas of science—from energy conversion and transport in advanced materials to biological processes and quantum information dynamics. Traditional experimental techniques often fail to capture these rapid, transient behaviors and the subtle structural

fluctuations intrinsic to these systems. Such experimental capabilities are essential drivers for theoretical developments in out-of-equilibrium physics that move beyond the mean-field approximations commonly used today. STS will help reveal fundamental mechanisms and drive theoretical understanding of nonequilibrium behaviors, ultimately leading to transformative discoveries in energy technologies, quantum computing, and life sciences.

3D strain tomography with microscale resolution: Researchers will be able to map complete strain tensor volumes with micrometer precision. This crucial capability will enable characterization and eventual manipulation of internal stress during additive manufacturing (AM). It will support the development of AM methods that can be routinely used to produce safety-critical components for the nuclear and aerospace industries, ensuring mechanical integrity.

Ultrashort timescale neutron studies: STS will advance the investigation of quantum materials, dynamic and kinetic processes, and complex systems in ways previously unattainable. It will mark a shift from static “snapshots” to dynamic “movies” in neutron research. This capability will allow researchers to monitor quantum state propagation and determine coherence and decoherence under in-use conditions across materials, interfaces, and devices.

Together, these features and capabilities position STS as the world’s most capable cold neutron scattering facility and will make STS the world’s most advanced neutron source, allowing researchers to address previously inaccessible scientific challenges and driving discovery in fields ranging from quantum information science to advanced manufacturing and energy technologies.

2.3 AI-ENABLED DISCOVERY, GENESIS, AND THE STS DATA ADVANTAGE

The rapid advance of AI has already reshaped how science is conceived, executed, and translated. To sustain U.S. scientific leadership, the next generation of major user facilities must do more than produce frontier data—they must be designed to operate as AI-ready discovery platforms. STS is being developed with this intent, aligned with the Genesis mission to accelerate autonomous, data-driven research at scale. By coupling unprecedented neutron performance with a modern data and compute ecosystem—including secure, federated capabilities envisioned through the American Science Cloud—STS will enable users to rapidly move from data collection to decision-grade inference reproducibly across institutions and facilities.

Instruments at STS will capture structural and spectroscopic information with unprecedented fidelity, driven by higher brightness (enabling finer time-of-flight resolution), next-generation detector pixelization, and high-throughput acquisition. The resulting step-change in measurement quality and volume will create a uniquely valuable data lake of world-class, multimodal neutron datasets. When paired with machine-actionable metadata, streaming pipelines, and scalable compute resources—capabilities central to Genesis and the American Science Cloud—STS will provide the enabling platform for training and validating a new class of science-specific models, surrogate models, and digital twins, delivering AI acceleration for challenges spanning biosecurity, next-generation manufacturing, and quantum materials for computing.

Surrogate models are computationally efficient approximations of complex physical systems that enable rapid simulation, optimization, and uncertainty-aware exploration of parameter space, while digital twins are continuously updated virtual representations of physical systems that integrate experiments, simulation, and machine learning to provide predictive insight under changing conditions; STS data will transform how both are built and used. High-resolution, time-resolved neutron measurements will

improve predictive accuracy, reduce model-form uncertainty, and enable near-real-time model updates during experiments, providing the technical basis for closed-loop experimentation in which models guide measurements, measurements refine models, and decisions converge rapidly toward scientific and engineering objectives.

Together these capabilities complement the Genesis mission by providing users with a faster, more reliable path from experiment to discovery through scalable, analysis-ready datasets and rapid inference that reduce time to insight, while standardized, auditable workflows strengthen reproducibility and confidence in results. By enabling uncertainty-aware experimental design and adaptive data acquisition, users can optimize beam time in real time and focus measurements where they matter most. The same infrastructure accelerates validation and translation by supporting rigorous studies under realistic, operando conditions, and it creates the high-fidelity, multimodal neutron data needed to train and benchmark next-generation foundation models that amplify scientific impact across the user community.

2.4 RECENT ORNL AI ADVANCES THAT ARE ENABLING NEUTRON SCATTERING RESEARCH

ORNL is already a world leader in applying AI/ML to neutron scattering, with advances that are transforming analysis, enabling real-time interpretation, and laying the groundwork for autonomous beamlines. These developments are directly aligned with the Genesis mission vision of scalable autonomy: integrating data capture, rapid inference, and automated decision-making into end-to-end scientific workflows. At FTS, scientists have developed AI tools that accelerate the modeling of inelastic neutron scattering (INS) data, reducing analysis times from days to minutes (Figure 8), enabling feedback during experiments, and supporting the next step toward automated experiment execution (Cheng et al., 2023). These AI-enabled workflows are expanding the accessible science space, including the analysis of anharmonicity driven by nuclear quantum effects that was previously beyond the reach of conventional approaches (Linker et al., 2024).

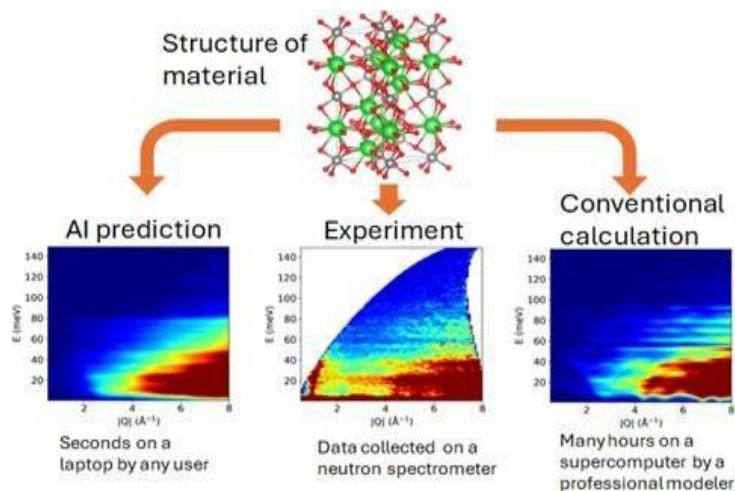


Figure 8. Structure of material. Schematic example showing how FTS AI models predict INS data in seconds, matching experiments and avoiding days of conventional computation.

AI is also delivering impact in SANS, where ML frameworks (e.g., Gaussian process regression) are being used to interpret scattering from complex soft matter and polymer systems. By leveraging synthetic datasets generated via high-performance computing, these approaches reduce dependence on restrictive analytical models and enable robust mapping of 3D structures, providing insight into systems such as functional copolymers where conventional methods can struggle.

Looking ahead, the scientific demand for speed, scale, and complexity increasingly requires high-throughput, autonomous experimentation. AI agents with adaptive learning and real-time experiment steering will be central to this evolution. STS is uniquely positioned to capitalize on ORNL's leadership-class computing capabilities (including Frontier) to generate high-quality training data, co-optimize experiments with simulation, and operationalize AI-enabled workflows for users through Genesis-aligned infrastructure and the federated access model envisioned by the American Science Cloud.

Two examples illustrate this trajectory. HyperCT (Tang et al., 2024) is an autonomous imaging system that optimizes scan strategies in real time, reducing measurement time nearly fivefold and dramatically increasing throughput. This approach anticipates key needs for STS-era real-time diagnostics and adaptive acquisition. ImagineX develops automated AI agents that build models through real-time data collection coupled to high-performance computing, enabling automated structural solutions and high-fidelity prediction of hydrogen positions in proteins. These capabilities essential for understanding biomolecular function and interactions relevant to therapeutic development.

2.5 STS COMPLEMENTS ORNL'S EXISTING NEUTRON SOURCES

ORNL is home to two world-leading neutron science facilities: SNS and HFIR. STS is the third pillar of the laboratory's 3-Source Strategy.

- FTS focuses on science that requires thermal and cold neutrons and provides sharp temporal resolution for the highest precision measurements of atomic-scale phenomena.
- HFIR is optimized for isotope production and measurements that benefit from the highest time-averaged flux of neutrons.
- STS will support research that demands high-brilliance cold neutrons, which are ideal for very small samples, dynamic systems, broad ranges of length and time scales, and high-resolution, data-intensive studies.

STS will enable the development of advanced next-generation instrumentation that complements the suite at FTS and HFIR. STS, designed for 21 instruments, will bring ORNL's total neutron instrument count to 54.

HFIR (6 cycles per year) and FTS (2 MW and 5000 h) together are capable of executing approximately 1,500 experiments annually. Each facility is oversubscribed by more than double on average; some programs are oversubscribed by a factor of five. Since the fuel event at the NIST Center for Neutron Research, which required a multiyear shutdown and cleanup operation, ORNL's facilities are the only open neutron user facilities available in the United States.

A fully instrumented SNS complex (FTS and STS) will provide approximately 8000 instrument days for the community. Completion of the HFIR Beryllium Reflector Replacement project will provide another approximate 2000 instrument days, bringing the total to about 10,000 instrument days, enabling approximately over 3000 annual experiments and the ability and capacity to support the growing user community demand for beamtime.

The current FTS instrument suite is scientifically the most productive of any operating neutron scattering center, with an average of over 17 peer-reviewed publications per year per instrument. The reference instrument suite at STS will provide an average gain factor of more than 100 over the FTS instruments.

These gains do not account for the discovery accelerations and efficiencies delivered by AI. The ORNL neutron scattering suite is co-located with world-leading high-performance computing and AI capabilities. Researchers at ORNL have already transformed the interpretation of neutron scattering data by applying state-of-the-art computational modeling, atomistic simulations, and AI/ML. Thus, ORNL is positioned at the forefront of automation and self-driving experiments. These developments will continue and will be directly applicable to the research conducted at STS, further accelerating scientific discovery.

The general reference suite instrument performance at STS will fulfill the stringent requirements of the grand challenge areas identified by the scientific community. These grand challenge areas are considered in the following sections.

3. PRIORITY RESEARCH DIRECTIONS TO ADDRESS STS SCIENTIFIC GRAND CHALLENGES

The following sections describe the scientific grand challenge priority research directions identified by the U.S. science and technology community as both pressing and requiring new neutron scattering capabilities to address. During a two-day workshop, followed by subsequent short meetings and town halls, representatives from the U.S. research community discussed the critical science needed in their fields for the United States to maintain leadership. The science areas are organized in broad themes: quantum materials, materials engineering, advanced chemistry and catalysis, soft matter and polymers, and biological systems. The priority research directions in each section were chosen from the broader community needs as outstanding examples that showcase the transformative science potential of STS and indicate science areas that genuinely require the capabilities of a next-generation neutron facility.

4. QUANTUM MATERIALS FOR FUTURE SCIENCE AND TECHNOLOGY

Quantum materials are critical for the future of science and technology, offering the potential to revolutionize key technologies, including quantum computing, quantum sensing, energy harvesting, and energy systems. Their unique properties, emerging from the complex interactions between charge, orbital, spin, and lattice degrees of freedom, drive breakthroughs in these fields. The surging demand for computation requires accelerated discovery of next-generation quantum materials. As recognized in the National Quantum Initiative Act and in recently passed federal regulations, quantum materials will be key to U.S. technological leadership and global competitiveness in the post-silicon era.

Neutron scattering is an essential tool for quantum materials research because it has the unmatched ability to quantitatively elucidate static and dynamic magnetism. Magnetism in quantum materials is of fundamental importance to realize and understand exotic ground states and provides a path to next-generation, energy-efficient quantum devices with broad applications in spintronics, quantum computing, sensing, and communication.

Today's neutron sources can identify candidate quantum materials of interest and are an important component of the discovery pipeline. However, quantum materials prediction and discovery are progressing rapidly, and providing the unique information that can be obtained only from neutron scattering at a necessary pace to fill an essential role in the prediction–synthesis–characterization cycle requires transformative capabilities. STS will fill this capability gap, revealing the nature of quantum ground states and providing unique understanding of quantum coherence and entanglement in small quantities of newly synthesized materials.

As quantum materials are incorporated into devices, it is essential to understand whether the expected quantum states persist and remain coherent in device formats and in the presence of interfaces. INS can provide unique understanding of the nature of quantum ground states, coherence of these states, and the

degree of quantum entanglement in a material. Unfortunately, today's neutron instruments cannot perform these measurements on thin films, as would typically exist in devices, because of intensity limitations.

The world-leading peak brightness of STS will overcome this limitation, enabling the first routine INS experiments on heterostructures and providing essential information on quantum devices. By providing this information, STS will play a critical role in engineering longer-lasting and error-free quantum state propagation or readout, will provide insights into material defects and instabilities—particularly at interfaces that are important for novel quantum devices—and will help to drive the development of materials for the next generation of U.S. quantum platforms, including quantum computing.

Over the past few decades, quantum materials have led to significant advances in computation and energy efficiency. Notable examples include giant magnetoresistance for magnetic storage (2007 Nobel Prize in Physics) and blue-light LEDs for lighting (2014 Nobel Prize in Physics). However, the growing demand for computation requires the accelerated discovery of next-generation quantum materials. STS will allow imaging of the complex interplay between degrees of freedom in quantum materials with unprecedented fidelity, accelerating understanding and applications of the associated collective phenomena. The following sections describe two priority research directions and the critical role that STS will play at the intersection of fundamental and applied science in quantum materials.

Impact of STS on Quantum Materials Research

Neutron scattering provides an unprecedented understanding of the structure and dynamics of magnetic materials due to the dipole interaction between the neutron spin and magnetic moments in materials. The world-leading cold neutron brightness at STS combined with the broad bandwidth provided by 15 Hz operation will provide transformative capabilities to elucidate the fundamental properties of quantum magnetic materials.

STS neutron spectrometers: Time-of-flight (TOF) neutron spectrometers efficiently explore broad ranges of wavevector and energy, and the resulting data can be quantitatively analyzed to extract fundamental interactions in materials. Neutron spectroscopy is the only technique that can quantitatively extract $S(Q, \omega)$ at millikelvin temperatures, providing essential understanding of quantum states of matter. Using cold neutrons, these data can be studied with energy resolutions as low as tens of microelectronvolts. The two classes of TOF spectrometers are direct geometry (fixed incident energy) and indirect geometry (fixed final energy) spectrometers. STS will enable the development of world-leading spectrometers of both classes. In addition to the STS peak brightness combined with modern focusing optics, the 15 Hz operation will enable direct geometry spectroscopy to simultaneously measure up to eight incident energies. These improvements combine for an overall performance increase of at least 80× compared with today's best direct geometry spectrometers. Although direct geometry instruments provide the most comprehensive mapping of wavevector and energy, indirect geometry spectrometers can provide unprecedented incident flux for a more restrictive wavevector range. At STS, such spectrometers will enable measurements from crystals with a mass of tens of micrograms, more than three orders of magnitude less than what can be measured today. At both the ISIS facility in the United Kingdom and the ESS in Sweden, plans are underway to construct next-generation spectrometers focused on small sample measurements, but the planned STS spectroscopy suite will outperform international competition and provide unique capabilities.

Polarization: Polarized neutron spectroscopy and diffraction can provide unique information to allow researchers to understand complex quantum magnets. Such measurements result in significant intensity reductions due to the inherent loss of half of the incident neutrons and because of the efficiency of polarizing optical components. Additionally, extracting the most general information requires multiple measurements with different field orientations. For example, while spin-polarized inelastic neutron scattering is—in principle—possible today, intensity limitations mean that the most general information

can be obtained only in highly idealized cases. The enhanced performance of STS spectrometers will make such experiments routine. This capability combined with polarized diffractometers at STS will provide critical information to compare with theory and to provide unique understanding of quantum entanglement in materials.

Extreme sample environment conditions: Applied pressure can change the fundamental interactions between magnetic moments by altering interatomic distances, and this phenomenon can be used to tune novel quantum states. The maximum available pressure increases with decreasing sample size; consequently, STS instruments optimized for measuring small samples will enable both spectroscopy and diffraction experiments at unprecedented pressures. Combining this capability with low temperatures will provide transformative insight into the nature of pressure-induced quantum states.

Neutron scattering is an essential tool with which to study magnetic materials, so the natural desire is to perform such experiments in the presence of applied magnetic fields. Unfortunately, the maximum magnetic field available for neutron scattering has not increased for about 30 years (National Academies of Sciences and Medicine, 2024). Increasing this maximum field allows for neutron scattering studies with an expanded parameter space and can drive quantum systems close to magnetic saturation where their properties become more classical in nature. Pushing beyond current limits requires new magnet designs together with infrastructure to minimize the impact on nearby instruments and equipment. This configuration cannot be accommodated at either of ORNL's existing neutron sources and requires a dedicated facility at STS. Furthermore, for vertical field split coil magnets, achieving the highest fields requires the smallest split between the coils; therefore, STS's ability to measure small samples will enable the highest fields. High magnetic field spectroscopy at STS will provide unique understanding of materials with fractionalized quasiparticles, which can be driven close to magnetic saturation, and the resulting excitations can be analyzed using classical methods.

Thin-film structure and dynamics: Functionalizing quantum materials often requires thin films, and understanding how the properties of these materials evolve in the presence of interfaces is of fundamental importance. STS will provide world-leading instrumentation for diffraction, polarized reflectometry, and even spectroscopy studies of thin films, providing essential information about the structure and dynamics of thin films of quantum materials. STS spectrometers will enable INS measurements from 10–100 nm thin films, allowing researchers to study the effects of interfaces on fundamental quasiparticles like spin waves, phonons, and spinons.

Box 4.1 Signature STS Capability: Neutron Spectroscopy Studies of Thin Films

The ability of neutron scattering to investigate the fundamental properties of bulk magnetic materials is unmatched. Because of their limited sample mass, thin-film sample measurement modalities are currently limited to neutron reflectivity and diffraction. These probes measure the depth-dependent magnetization or microscopic arrangement of magnetic moments; however, the fundamental understanding of magnetic interactions provided by INS has remained out of reach for thin-film samples. STS will enable these measurements for the first time and establish entirely new thematic science programs. These studies can be undertaken at millikelvin temperatures with 10–100 μeV energy resolution and excellent Q resolution, providing a unique experimental modality. This capability will provide access to $S(Q,\omega)$ from thin films in a parameter space that is crucial for quantum magnets, strongly correlated materials, and novel superconductors.

The new class of indirect geometry neutron spectrometers that will be available at STS will enable leadership in an environment where European facilities (ISIS and ESS) are moving toward the development of spectrometers to enable measurements from small samples and thin films. The development of such instrumentation at ORNL requires the STS source and will combine the 10 \times brightness increase of STS, advanced focusing optics, and the inherent gain factor of >50 for indirect spectrometers to enable the measurement of samples with mass of tens of micrograms. Such an instrument at STS would outperform proposed instruments at ESS and ISIS, providing world-leading capabilities to U.S. researchers.

STS indirect geometry spectrometers will enable investigations of thin-film samples that are 10–100 nm thick with an area of 1 cm^2 . For quantum magnetic materials, this capability will enable transformative experiments to reveal how magnetic excitations and quantum states evolve in stacked layers. This signature capability will open the possibility to measure magnetic excitations in thin films and patterned structures as a function of both vertical and lateral confinement, where finite size and interface/surface effects are strong.

Certain materials, such as some nickelate superconductors, cannot be synthesized as bulk crystals and can be produced only as thin films. STS will be the first facility to enable studies of the spin dynamics of these types of systems with the required resolution and at ultralow temperatures. INS from thin films at low temperature and with high resolution also opens exciting possibilities to investigate hybrid excitations at interfaces between dissimilarly ordered magnetic materials.

The consequences of lattice strain on thin film materials are the subject of intense study. INS on thin films will enable studies of lattice strain effects on their quantum behavior and provide direct measurement of differences in $S(Q,\omega)$ in thin films and bulk materials. Strain directly affects the interatomic spacing and commensurately the magnetic interactions of thin-film materials. INS studies of thin films will facilitate the development of theoretical models of strained spin systems and provide understanding of the fundamental quantum properties in confined geometries relevant to next-generation quantum devices.

4.1 GRAND CHALLENGE 1: DISCOVER QUANTUM MATERIALS THAT APPROACH FUNDAMENTAL LIMITS FOR INFORMATION AND ENERGY TECHNOLOGIES

Key Questions

- Can we develop an accelerated quantum materials discovery program with neutron scattering serving as an essential experimental ground truth?

- Can neutron scattering provide fundamental information on small early-production quantities of materials, enabling the screening of new materials?
- Can neutron scattering studies of materials at unprecedented extremes of temperature, magnetic field, and pressure provide unique insights into the properties of emerging quantum materials?

A vast space of quantum materials awaits discovery, with potential applications in dissipationless interconnects, topological quantum computing, spin-based information transmission, and energy scavenging. Although predictive models of material properties from atomic-scale structural information have significantly improved, especially with programs like the Materials Genome Initiative, the next quantum revolution demands predictive capabilities specific to quantum materials. These capabilities will underpin a comprehensive materials discovery program.

To efficiently explore the quantum materials landscape, AI and ML tools will be essential, replacing manual processing and deterministic algorithms. However, these AI-driven programs will require vast amounts of data, gathered from direct probes of quantum states of matter. Given that static and dynamic magnetism are central to quantum material properties, neutron scattering will play a pivotal role in this revolution, and STS will provide the necessary data rates to support these advancements.

The functionalization of candidate quantum materials will also depend on thin-film form factors. The interfaces formed between quantum materials present rich opportunities for creating new electronic functionalities. With the brightness of STS, depth-resolved characterization of magnetic structures and dynamics in samples closely resembling real device configurations will be possible, facilitating the understanding and development of these materials.

4.1.1 Accelerating Discovery of Functional Quantum Materials

The increase in cold neutron brightness at STS, combined with a full range of instrumentation, will increase data rates by two to three orders of magnitude. With these improved rates, AI-guided decision-making and real-time information extraction can be employed during experiments (Chen et al., 2021).

Quantum materials discovery will benefit from accelerated AI-informed discovery workflows, detailed investigations of material functionality under external stimuli and extreme conditions, and measurements of spatially confined and driven excitations in quantum materials.

The discovery of new quantum materials typically involves an iterative cycle of prediction, synthesis, and characterization (Giustino et al., 2020). Growing international interest in quantum information science has rapidly increased the pace of prediction and synthesis of new materials, and AI-driven tools are poised for further acceleration. Completing this cycle requires vast quantities of high-quality experimental data.

Neutron scattering provides unique understanding of the nature of quantum ground states and can be quantitatively compared to theory, modeling, and simulation. Neutron scattering data can serve an essential role in completing the prediction–synthesis–characterization cycle, but current capabilities require large samples, and investigations are often performed long after initial sample synthesis. The enhanced brightness and broad bandwidth of STS will produce neutron data at rates that match advances in modeling and synthesis, accelerating the discovery process. STS will also enable faster and more comprehensive measurements of new materials, even when only small quantities are available. This capability will facilitate a quicker feedback loop between theoretical predictions, synthesis, and experimental validation, significantly shortening the time needed to identify promising materials and advance their development for real-world applications.

Understanding the physics at surfaces and interfaces is essential for the complete description of materials and for enabling theoretical predictions of quantum material functionality. Topological quantum materials, for instance, can feature symmetry-protected edge states on their outer layers; these states have very long lifetimes. Orders of magnitude more flux at STS will enable INS from thin-film heterostructures, allowing studies of the influence of interfaces on fundamental quasiparticles such as spin waves, phonons, and spinons. The brightness of STS will also enable polarized neutron reflectometry from surfaces as small as 1 mm² in a single instrument configuration, allowing for time-dependent studies of driven devices.

Antiferromagnetic spintronics devices hold tremendous potential to increase the speed, density, and energy efficiency of electronic information storage systems. Developing and optimizing materials and structures for such applications require an understanding of antiferromagnetic spin structures and dynamics in driven devices. The current state-of-the-art probing methods are limited to spin-polarized scattering-length densities, and data interpretation remains model-dependent, thereby limiting the development of predictive theoretical models. Instruments at STS will allow researchers to use additional atomistic probes, such as INS, to investigate spin diffusion and spin switching, aiding theoretical development and understanding. This capability, in turn, will enable next-generation microelectronics that use spin rather than charge, increasing device speed and reducing device size.

4.1.2 Revealing Novel Properties of Quantum Materials Under Extreme Conditions

Quantum materials' unique responses to external stimuli, including electric and magnetic fields or light, form the basis of their applications. AI-driven methods will improve the ability to predict these functionalities. Verifying predictions and elucidating how functionalities emerge in quantum systems require detailed studies under varied experimental conditions. The intense, focused beams at STS will enable comprehensive parametric studies of large families of new materials that are available only in pilot-scale quantities. These studies will extend to materials under extreme conditions of temperature, pressure, and magnetic field, where large samples cannot be measured.

Roughly one out of every five neutron scattering experiments on quantum materials is conducted under applied magnetic fields. Combining neutron scattering with high magnetic fields provides unique insights into mechanisms and functionalities. Stronger magnetic fields allow exploration of expanded phase spaces and a broader range of energy scales. However, no progress has been made in increasing the maximum field available for neutron scattering in the past 30 years (National Academies of Sciences and Medicine, 2024). To maximize scientific impact, the world's brightest neutron source should be paired with cutting-edge magnetic fields: steady fields exceeding 30 T and pulsed fields exceeding 50 T. These fields require specialized magnet installations designed for optimal neutron performance while minimizing interference with other beamlines. These advanced installations cannot be achieved at existing ORNL neutron sources; they can be realized only at STS.

Box 4.2 Transforming Our Ability to Understand Bulk and Thin-Film Quantum Spin Liquids

One of the biggest challenges in quantum technology is quantum decoherence, which disrupts the fragile quantum states necessary for devices to function. To counter this phenomenon, scientists are exploring ways to make qubits more robust, either by improving their design or by using error-correction techniques. A more advanced approach involves creating new materials with inherent resistance to decoherence. Quantum spin liquids (QSLs) are an exotic, topological, condensed matter phase characterized by emergent fractionalized quasiparticles and long-range entanglement. As such, QSLs are a promising candidate for fault-tolerant stable quantum information devices. STS will enable experiments that were previously impossible, providing U.S. researchers with a critical advantage in identifying and functionalizing quantum materials such as QSLs.

The challenge to understand the physics that drives quantum decoherence—which fundamentally disrupts the fragile quantum states necessary for quantum devices to function—can be addressed by performing highly sensitive INS experiments at STS. Measuring the signals of interest, defined excitations in wavevector and energy transfer as well as broad continua of scattering, require highly sensitive instrumentation with excellent signal-to-background resolving power. The peak brightness, bandwidth, and facility characteristics of STS will vastly improve our ability to study excitations across broad ranges of wavevector–energy space. This capability will enable studies of dispersions and lifetimes of both magnetic and lattice excitations simultaneously, with far greater sensitivity than is currently achievable, providing unique insight into QSL decoherence pathways.

Candidate materials may exhibit long-range magnetic order at the lowest temperatures and must be driven by external parameters such as applied magnetic field or pressure to achieve a QSL state. Small sample volumes are necessary to reach extreme values of applied pressure and magnetic field. The peak brightness of STS will enable quantitative studies of magnetic structure and dynamics from very small samples, enabling studies at unprecedented pressures. The facility characteristics will enable co-design of neutron scattering instrumentation and high magnetic field environments with fields >30 T. These experimental capabilities can be used to understand the phase diagram of candidate materials and elucidate the physics of quantum and classical states. High magnetic field INS measurements, during which the material is driven to a field-induced, classical state, can reveal the fundamental spin interactions in QSL candidates.

After identifying and characterizing the most promising materials, it is important to observe how these properties evolve in the presence of interfaces that would be present in a real device. STS will enable neutron spectroscopy measurements from 10–100 nm films, revealing how magnetic excitations evolve in stacked layers and in the presence of interfaces.

The combination of STS capabilities will be transformational in our ability to identify candidate QSL materials and understand their fundamental properties, the stability of the QSL state, and how the properties evolve in the presence of interfaces. The potential impact of QSLs could be profound: if a stable, tunable, and controllable QSL system with novel (non-Abelian) quasiparticles can be fully realized, then QSLs may underpin a next-generation quantum computing architecture that is fundamentally more robust than today’s noisy intermediate-scale quantum systems.

The Hamiltonian of a quantum system describes the energy scales of all relevant interactions. Neutron scattering in magnetic fields greater than 30 T will be possible at STS with next-generation superconducting magnets. Coupling large magnetic fields to neutron scattering instrumentation with the intense cold neutron beams of STS will provide a unique capability, enabling unambiguous determination

of the underlying Hamiltonian in various quantum magnets. For example, magnetizing a material with topologically protected states, such as the Kitaev magnet α -RuCl₃, combined with neutron spectroscopy at STS, will allow for full determination of the underlying spin Hamiltonian—a challenge that remains unresolved. This capability will enhance efforts to understand and exploit quantum spin liquids (QSLs) for topological quantum computing.

Pressure alters interatomic distances and shifts the energy scales of interacting magnetic moments, revealing novel quantum states of matter. The unmatched peak brightness of STS will enable unique high-pressure capabilities: inelastic scattering to probe spin dynamics under pressures up to 30 GPa and detailed neutron diffraction studies at pressures up to 100 GPa. Combining these capabilities with low temperatures will be crucial for understanding pressure-induced quantum states.

4.2 GRAND CHALLENGE 2: ADVANCE UNDERSTANDING OF QUANTUM COHERENCE AND FUNDAMENTAL DYNAMICS IN MATERIALS PLATFORMS

Key Questions

- How can quantum decoherence be overcome in the application of new quantum materials?
- Can fundamental properties like quantum entanglement be quantitatively understood, providing an experimental measure of “quantumness”?

STS will dramatically expand the dynamic range and sensitivity of neutron scattering across the length and time scales needed to advance the characterization of quantum materials. The physics of quantum states of matter often lies in the quasiparticles they support. Examples include Bogoliubov quasiparticles, spinons, Majorana fermions, visons, and magnetic monopoles. These particles reveal mechanisms behind magnetically mediated superconductivity and form the foundation for applications ranging from information and heat transfer to quantum computing. INS is the principal method for detecting quasiparticles, and the transformative capabilities of STS will enable measurements on minuscule quantities of high-quality material under extreme thermodynamic conditions, in confined nanostructures, and beyond thermal equilibrium.

Coherent quantum states are long-lived; however, external perturbations can disturb these states, leading to a return to the decoherent classical or ground state. Experimental studies of materials exhibiting quantum coherence and decoherence are crucial for advancing our understanding of the transition between the quantum and classical domains. Neutron studies will help develop the ability to manipulate such states, driving the development of new material platforms for quantum information technologies.

The improved dynamic spectral range and sensitivity of INS at STS, combined with polarization analysis, will enable the study of foundational aspects of quantum theory. In particular, understanding the quantum-to-classical transition remains tenuous. To characterize these systems and manipulate these states effectively, quantitative probes are required. Neutron scattering is an ideal quantitative probe of quantum systems. Decoherence effects, which limit the capabilities of quantum computers, are of particular interest. STS will serve as a quantum laboratory, providing insights into how decoherence can be controlled, ultimately improving quantum computing performance. The superior resolving power of STS will make the quantum-to-classical crossover in quantum materials more accessible.

4.2.1 Unlocking Fundamental Insights into Quantum Materials

The enhanced source brightness and novel instrumentation concepts at STS will provide cold neutron spectroscopy with the required resolution and sensitivity. For example, in the quest for QSLs, improved measurement resolution will offer spectroscopic access to the crossover between QSL behavior and lower

energy regimes, where material-specific defects or weak interactions induce decoherence, spin freezing, or magnetic ordering. More precise measurements will accelerate the quantum materials optimization process and drive progress from materials to devices.

Magnetic materials frequently develop conventional types of long-range order, such as ferromagnetism or antiferromagnetism. Spin liquids (Figure 9) have more complex forms of order, with emergent excitations. New materials such as NaYbSe_2 are promising possibilities that appear to lie beyond conventional order. Gapless spin liquids, with excitations that can exist at near-zero energy and without long-range order, fall beyond established theories of topological order. Additionally, gapped spin liquids could appear gapless because of defects or an intrinsically small gap. Measuring wavevector-dependent spin correlations in the ultralow energy regime is essential for determining the nature of such materials.

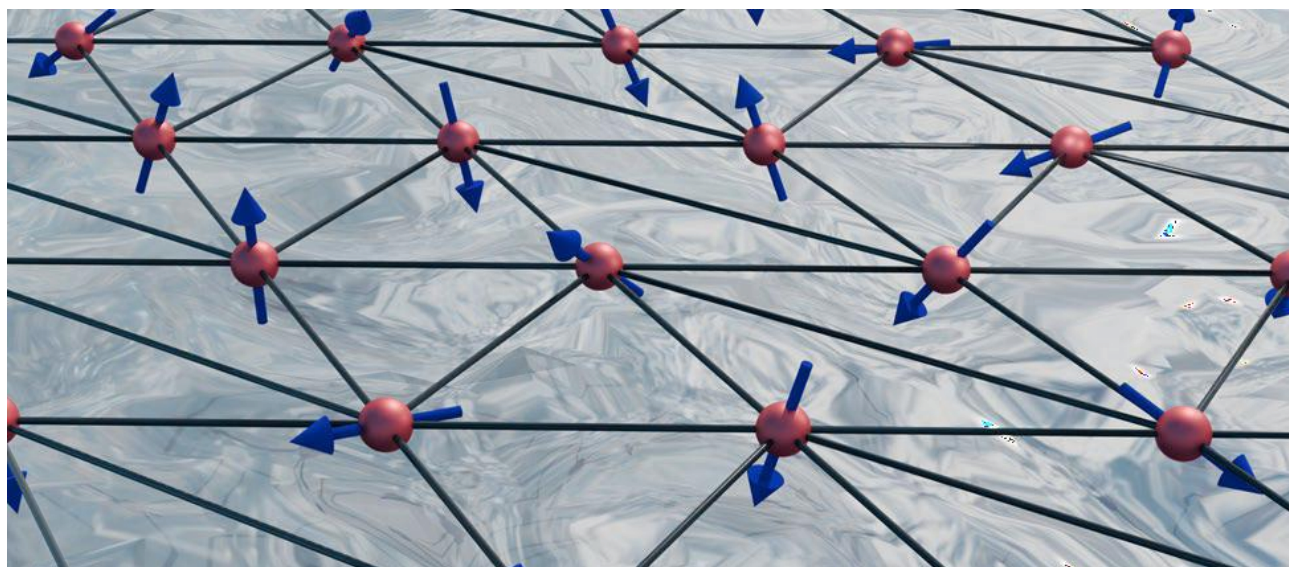


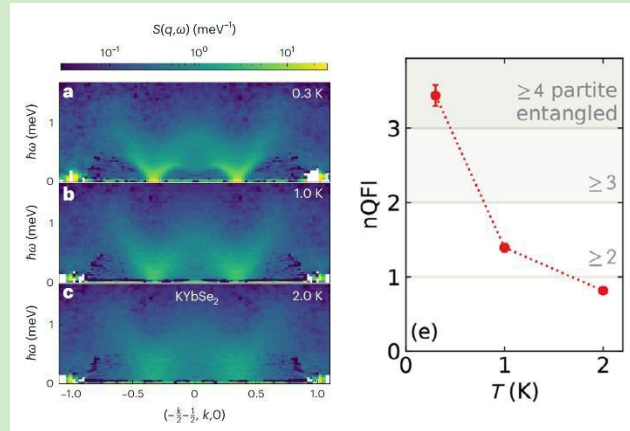
Figure 9. Schematic image representing the fluctuating and entangled spin interactions of particles in a QSL. Here, the spins remain disordered and dynamic at quantum levels, exhibiting liquid-like behavior. *Image courtesy Theresa Ahearn/ORNL.*

Fully spin-polarized INS is an incredibly powerful probe. Although technically possible today, current intensity limitations and the requirement to measure multiple field orientations make such measurements feasible only in idealized cases. The brightness of STS, combined with fully optimized instrumentation, will make these experiments routine, providing critical and unique data for theory comparison and quantum calculation testing.

A model-independent determination of solid-state quantum entanglement remains a persistent challenge. An emerging approach involves extracting entanglement witnesses from the two-point correlation function, which can be directly measured by INS. Full polarization analysis will bring out the full potential of this method. STS will uniquely enable this capability, providing a versatile, quantitative gauge of quantumness in materials.

Box 4.3 Quantum Entanglement Witnesses

Quantum technologies fundamentally depend on entanglement—a phenomenon in which two or more particles cannot be described independently, even across large distances. To develop the most promising materials for these technologies, it is important to extract quantitative, model-independent measures of entanglement.



On the left, INS measurements of KYbSe₂ at different temperatures (from the CNCS spectrometer at SNS) as a function of energy (vertical axis) and momentum transfer (horizontal axis). On the right, normalized quantum Fisher information at the ordering wavevector (Scheie et al., 2024).

One exciting approach that has emerged is the use of entanglement witnesses, concepts from quantum information theory applied to materials (Laurell et al., 2025; Scheie et al., 2025). Some of the most relevant entanglement witnesses, such as quantum Fisher information (QFI), a measure of multipartite entanglement, requires wavevector-dependent spectroscopy measurements. Unlike traditional approaches that require full knowledge of the quantum state, QFI can be accessed from neutron spectroscopy data in a model-independent manner. To extract QFI, excitations must be measured over an appropriate range of momentum transfer and energy transfer with sufficient energy resolution (from tens of microelectronvolts to millielectronvolts), and at low temperatures (often <1 K). Furthermore, the scattering technique must allow straightforward conversion of the measured cross section into a dynamical structure factor in absolute units. Cold neutron spectroscopy is the only technique that meets all these requirements. The figure shows neutron spectroscopy data and the extracted QFI from KYbSe₂ (Scheie et al., 2024) consistent the low-temperature emergence of a highly entangled quantum state.

The next-generation direct geometry spectroscopy instruments at STS will revolutionize our ability to probe entanglement in quantum materials. These instruments will offer at least an $80\times$ increase in performance compared to current FTS capabilities, which are already the best in the world. The STS 15 Hz operation will support simultaneous measurements with multiple incident neutron energies, allowing mapping of magnetic excitations with varying energy resolution. This enhanced STS capability will enable parametric studies of entanglement with improved accuracy, including routine use of polarized neutrons. Polarized measurements are essential to fully quantify entanglement in anisotropic systems and will open pathways to measuring additional entanglement-related quantities like nonlocality.

STS will make routine, accurate quantification of entanglement in quantum materials a reality, enabling researchers to quantify entanglement over broad ranges of phase space and identify ideal candidates for device applications. The ability to quantify entanglement across complex phase diagrams with higher fidelity will deepen our understanding of entangled states, paving the way for accelerated commercialization and technological innovation based on quantum materials.

4.2.2 Enabling Understanding and Control of Quantum Decoherence for Enhanced Functionality

Quasiparticles are analogous to classical particles because they have both momentum and energy; however, they are associated with excitations from an extended many-body state. Unlike traditional scattering measurements that focus on determining the presence of excitation energies, STS will enable detailed line-shape analysis to probe quasiparticle lifetimes. Characterizing these lifetimes helps reveal how quasiparticles interact and decay; this information is essential for understanding decoherence in quantum spin systems and improving materials.

The use of solids to create states with long-lived quantum coherence, such as diamond color centers or superconducting qubits, is of great importance. STS will offer the potential to study decoherence processes in solids at ultralow temperatures, covering the timescale from the initial interactions between an electronic or spin state and its environment to the emergence of classical dynamics. STS will uniquely enable such studies in complex interacting materials.

Thanks to its high brightness and time structure, STS will probe quantum materials driven beyond thermal equilibrium with currently unachievable time resolution. Understanding this physics is fundamentally important and essential for practical applications, which often operate away from thermal equilibrium. Research on how pulsed or time-periodic perturbations drive quantum materials into regimes with emergent physics is a critical and urgent area of study.

Materials with strongly interacting electrons exhibit collective properties driven by quantum mechanics. Understanding and controlling these novel states of matter present a major fundamental scientific challenge with exciting practical ramifications. Next-generation experimental capabilities with sensitivity to quantum properties, beyond what is possible today, are essential for progress. Neutron scattering—with its sensitivity to excited states at millielectronvolt energies, microelectronvolt resolution, and ability to simultaneously study ground and excited states without disturbing or heating the sample—is critical. The ability to detect magnetism and measure properties over critical length and time scales is essential.

STS will transform neutron scattering studies of quantum materials by providing essential information on the structure and dynamics of small quantities of new materials early in their discovery and from devices, supporting a quantum materials discovery program that leads to prototypes. STS will also enable, for the first time, routine neutron spectroscopy studies of thin films. This capability will provide key insight into how novel quantum properties evolve in the presence of interfaces, which is essential knowledge in the transition from bulk materials to devices.

STS will enable studies that are not possible today: neutron scattering at unprecedented magnetic fields and pressures, tuning exotic states and gaining quantitative understanding of underlying interactions, fully polarized INS for a unique understanding of entanglement, high-resolution measurements to study quantum decoherence, and observations of quantum materials across interfaces and beyond thermal equilibrium. These capabilities are essential to maintain U.S. competitiveness in the global race for quantum materials and technologies.

5. MATERIALS SCIENCE AND ENGINEERING AT THE SECOND TARGET STATION

An in-depth understanding of materials will provide the United States with a competitive edge in next-generation manufacturing technologies. STS will be a crucial capability complementary to other neutron and light sources, enabling in situ probes of products as they are being formed.

STS will be essential for meeting the urgent need for the development of advanced manufacturing and construction processes that will ensure American industrial leadership. These advancements will offer

families a new range of appliances, consumer products, and housing options. Neutrons from STS will reveal the underlying behavior at multiple scales of next-generation materials as they are formed, using advanced imaging and analysis techniques that provide a powerful new tool for accelerating development and deployment. For example, additive manufacturing, often referred to as 3D printing, has revolutionized the creation of bespoke components across a variety of applications.

Impact of STS on Materials Science and Engineering

STS capabilities will accelerate next generation manufacturing capabilities for the United States. The key challenge in materials science is understanding and controlling the multiscale behavior of complex materials under real-world conditions to enable advanced solutions in energy, manufacturing, and infrastructure. Ideally, STS will provide experimental capabilities that allow researchers to simultaneously measure structures across relevant length scales from angstroms to nanometers to millimeters. These types of investigations can only be achieved by developing multimodal instrumentation. Neutron scattering instruments that can measure, for example, residual strain and small angle scattering simultaneously provide a very wide dynamic range of structural information to be probed during operando experiments on large engineering components will enable accelerated identification of key material properties and understanding of the structure function relationship. The ESS instrument suite includes several instruments with such capabilities, the Beamline for European Engineering Research Materials provides simultaneous residual strain, texture mapping and imaging capabilities. Heimdal is a bispectral diffractometer that allows simultaneous measurement of diffraction and SANS data. The source characteristics of FTS do not lend themselves to the development of multimodal capabilities for operando investigations: the operational bandwidth of 60 Hz is too narrow to enable useful determination of SANS at an instrument length needed to simultaneously support diffraction. However, STS is the ideal source for such instruments in the United States: the high brightness and large bandwidth allow instruments to be realized for multimodal capabilities without the performance compromises seen at FTS.

These types of multimodal investigations are not possible at light sources for life-sized engineering components. Although high-energy X-rays ($E > 100$ keV) are penetrating and required for engineering studies at light sources, the scattering process kinematics cause Bragg diffraction at very low scattering angles, commensurately hiding any small-angle signal in the measured data. For certain materials of interest such as FeNi superalloys, light source measurements are hindered by the lack of scattering contrast between atomic species that have similar atomic number.

5.1 GRAND CHALLENGE 3: ACCURATE DIGITAL TWINS TO ACCELERATE DISCOVERY AND DEVELOPMENT OF NEW MATERIALS

Key Questions

- How can we improve multiscale characterization to create accurate and dynamic digital twin materials?
- How can we enable timely and reliable certification of new radiation-tolerant alloys for 21st century fission reactors and novel fusion energy systems is a strategic energy materials need for the United States?
- How can we enable timely and reliable certification of failure-critical aerospace materials and components is a strategic industrial and military defense need for the United States?

STS will address these materials-engineering questions by making it practical to measure real components under realistic conditions in real time, tracking microstructure, strain, texture, defects, and phase evolution as they develop enabling development of predictive models and digital twins that are anchored

to ground-truth high fidelity data. The STS high-brightness cold-neutron capability and broad bandwidth enable integrated, multiscale workflows that link atomic to mesoscale characterization (e.g., diffraction and small-angle scattering) with component-scale imaging to capture the coupled processes that govern performance, including crack initiation, damage accumulation, and environmentally driven degradation. By delivering time-resolved, statistically robust datasets across relevant length and time scales, STS provides the validation basis needed for uncertainty-aware digital twins and for accelerated, evidence-based qualification pathways. This capability supports timely certification of radiation-tolerant alloys for advanced fission and fusion systems and of failure-critical aerospace materials and components essential to U.S. industrial competitiveness and national defense.

A major challenge facing the nation is the development and deployment of science-based certification methods for new materials intended for use in complex, dynamic, and/or extreme environments. Many industries require new materials and components to be certified, relying on databases of in-service performance data generated primarily by trial-and-error approaches. A classic example is the qualification of materials for the nuclear power industry.

Materials used in pressure boundary applications must follow the American Society of Mechanical Engineers code qualification process, which mandates thousands of hours of high-temperature ($>300^{\circ}\text{C}$) creep data from multiple process heats of the material (McMurtrey and Messner, 2021; Nickel et al., 1982; Sham and Natesan, 2017). Consequently, every new material, as well as every new form or structure (whether an old or new material), must undergo this time-consuming, costly, and complex qualification process.

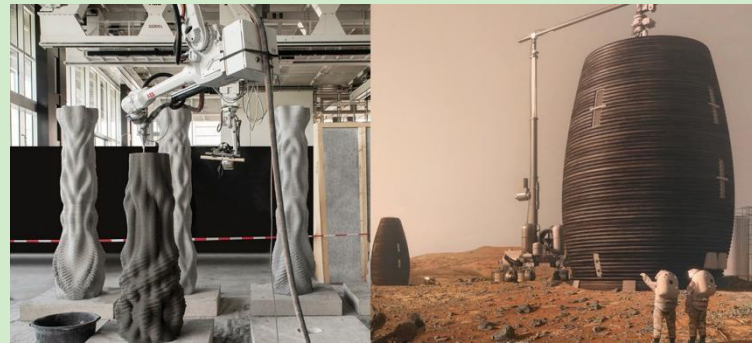
Despite recent advancements in materials design and manufacturing processes with engineered structures that offer superior properties and performance over existing materials and components, high-performance materials have not been deployed because they have not yet been certified or qualified. Moreover, new designs that require different shapes and structures are often discouraged, even though they could offer superior performance.

Consequently, reactor designers have been restricted to a small number of qualified fuels and materials that were certified decades ago, hindering the nuclear industry from employing the highest-performance materials. These outdated approaches stifle technological and energy progress due to the long lead times and often expensive nature of the exposures, particularly for materials, material systems, and components used in extreme environments.

A science-based approach for the certification of materials in engineering applications is to leverage digital twins—virtual tools that comprehensively encompass the formation/manufacturing process and the in-service performance of materials/components in four dimensions (i.e., the three spatial dimensions plus time). This paradigm shift will revolutionize the speed and efficiency with which new technologies can be brought to market, enabling rapid innovation and adaptation while considering safety, usability, recyclability, and other desirable attributes essential for fostering an energy-independent, resilient, and technologically advanced society. Digital twins represent a new and advanced tool that uses a library of experimental data verifiably linked to macroscopic effects. This causality is captured in a full digital model that is independent of shape or form, carrying information on in-use performance such as pressure, temperature, external magnetic or electric fields, and radiation.

Box 5.1. Constructing the Future: How Neutron-Driven Advances in Materials and Automation Will Transform Our Built World

Additive manufacturing and robotic construction could transform the built environment by shifting construction from labor-intensive, bespoke workflows to scalable, automated production. However, today's printable cementitious materials are still constrained by long and poorly controlled cure times, narrow processing windows (pumpability → extrudability → buildability), early-age cracking and shrinkage, and uncertain interlayer bonding. These limitations persist because the key chemical reactions and transport processes—hydration kinetics, phase evolution, moisture/ion migration, and stress development—occur within dense, aggregate-filled materials where critical interfaces are buried and evolve rapidly, making them difficult to measure directly. Polymer and soft-matter science is an equally important (and underdeveloped) lever for controllable printing. Many printable cements rely on polymeric or polymer-like additives—superplasticizers, viscosity modifiers, thickeners, dispersants, shrinkage-reducing agents, latexes, fibers, and emerging hydrogel concepts—to tune yield stress, thixotropy, water retention, setting rate, and interlayer “healing.” Yet we still lack predictive understanding of how these macromolecules adsorb to particle surfaces, mediate dispersion/flocculation, form transient networks, and reorganize as hydration progresses in highly ionic, reactive pore solutions. Without that structure–property map, formulation and process control remain largely empirical.



On the left, a robotic arm is seen 3D printing detailed concrete columns in a laboratory environment. On the right, a NASA concept depicts 3D printed structures being constructed on Mars for future human habitation. Source: NASA. 2023. “3D Printing for Mars Habitation.” NASA, accessed March 2025. ETH Zurich/Concrete Choreography.

STS and neutron science provide the measurement backbone needed to move from trial and error to predictive, certifiable additive construction. Bright cold pulsed neutrons can penetrate realistic specimens and are highly sensitive to water and hydrogen-bearing species, enabling time-resolved tracking of hydration, moisture redistribution, pore formation, and buried interfaces across nanometer-to-millimeter length scales. Combining neutron imaging/tomography with diffraction and scattering makes it possible to connect evolving microstructure and phase composition to early-age deformation, interlayer integrity, and fatigue-relevant damage—under realistic construction environments (temperature, humidity, applied loads, and curing conditions). With STS brightness, these measurements become fast enough to capture transient printing states and early-age curing in situ, producing “decision-grade” datasets. Looking forward, this capability is even more critical for off-planet construction, where structures must be built from locally sourced minerals with nonstandard and highly variable aggregate properties. Reliable lunar or Martian construction will require the ability to tune aggregate fraction, particle size distribution, and mineralogy along with binder and polymer/additive packages to achieve printable rheology, controlled setting, and durable interfaces under extreme thermal cycling and reduced gravity. STS-enabled neutron datasets can quantify how local minerals influence reaction pathways, interface formation, and curing kinetics, providing the experimental foundation to train AI models and implement closed-loop formulation and process control. In short, STS helps make autonomous additive construction practical on Earth by enabling predictable cure and bond performance and off-planet by enabling materials engineering from the minerals available at the build site.

Such a revolution in materials development and certification presents a grand challenge because of the complexity and interconnectivity of intrinsic and extrinsic factors that influence material performance. The interplay of material structure and composition with various stimuli during service, such as stress, temperature, pressure, magnetic fields, and electric fields, complicates this process. Even a small change in a single variable can significantly alter the immediate and/or long-term performance of a material.

Capturing the coupled correlation of composition, structure, and properties is inherently difficult, if not impossible, with current means and timelines for materials synthesis and interrogation. This grand challenge represents the culmination of over a decade of established priority basic research (Walck et al., 2024).

An example of the current state of the art in science-based certification is the ongoing effort toward the qualification of additively manufactured components. Presently, additively manufactured products are qualified based on simple test geometries that often overlook spatial and temporal variations in thermal and mechanical strain as well as the presence of physical defects. This process leads to standards that cannot quantitatively estimate component life. The materials community has been challenged to develop science-based qualification methods using computational modeling and in situ monitoring (e.g., DARPA's Structures Uniquely Resolved to Guarantee Endurance program). Early fracture detection in advanced components during the void nucleation phase remains the holy grail of engineering mechanics and requires the determination of microstructural features in bulk materials under load/temperature at nano- to microscale spatial resolution. These criteria could be met using dynamic cold neutron imaging at STS, coupled with Bragg-edge imaging analysis (for strain/phase evolution) and neutron grating interferometry modalities (for porosity–precipitate–microcrack evolution across a range of scales) (Chen et al., 2023). However, full realization is beyond the scope of current capabilities and facilities.

Figure 10 illustrates how neutron imaging techniques can resolve spatial variations in lattice spacing within a dual-column metallic sample, a foundational capability for real-time fracture detection and materials qualification. STS will advance this capability by delivering higher brightness cold neutrons and sharper TOF resolution, allowing for more precise Bragg-edge measurements, improved strain mapping sensitivity, and faster imaging rates essential for in situ monitoring of structural materials under load or during dynamic processes.

Timely and reliable certification of new radiation-tolerant alloys for 21st-century fission reactors and novel fusion energy systems, along with failure-critical aerospace materials and components, is a strategic need for energy and defense sectors in the United States. Early detection of defects and fractures in component-scale samples will be essential for tuning and benchmarking such numerical models to the point at which their results are of sufficiently high quality that they are accepted by certifying agencies in lieu of expensive parametric fatigue experiment series.

Multimodal cold neutron instruments at STS will enable live in situ or operando measurement of a variety of parameters under controlled conditions with sufficient resolution to test model predictions and generate accurate digital twins. STS-based SANS, imaging, and diffraction beamlines will provide data for key insights into the dynamics/kinetics under the relevant environment. The development of detailed digital twins for predictive modeling and real-time monitoring will accelerate the development of novel materials with amplified performance, safety, reliability, and longevity across various industries. By addressing the limitations of current certification processes, STS will drive innovation and support the transition to energy dominance and advanced technologies.

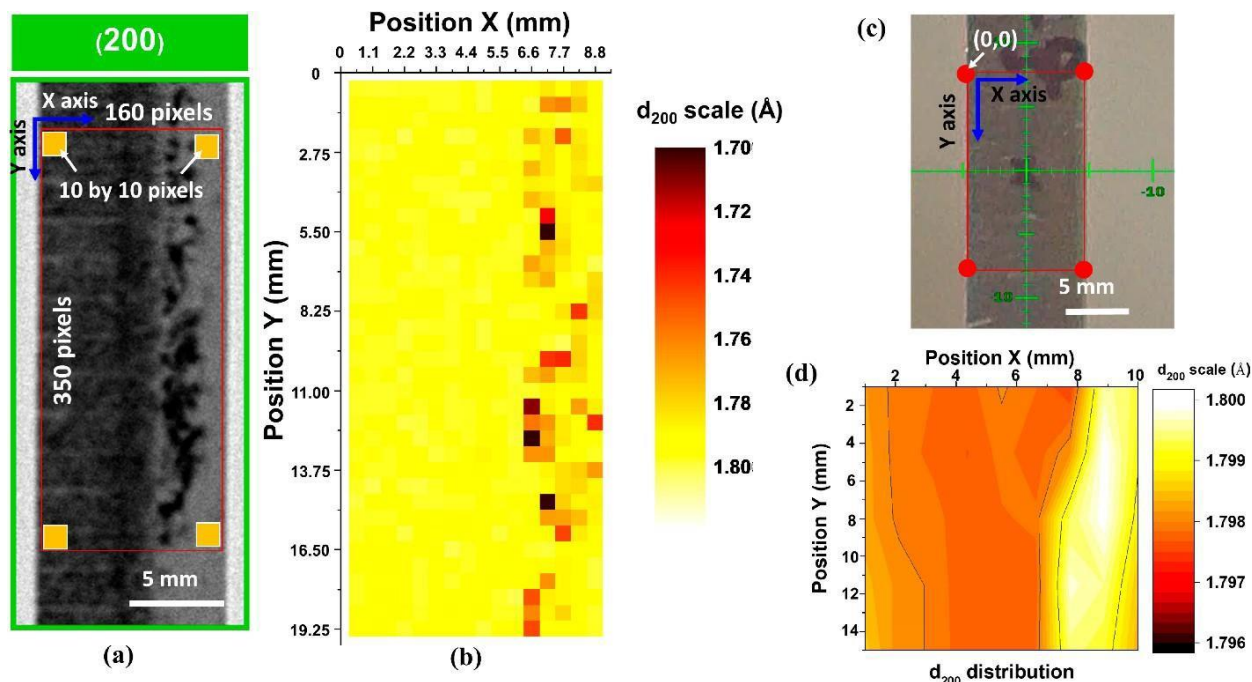


Figure 10. Neutron imaging techniques can resolve spatial variations in lattice spacing. (a) A (200) Bragg-edge radiograph with imaging data analysis details and (b) the distribution of the (200) interplanar spacing (d_{200}) for the dual-column sample (no loading) determined by iBeatles fitting. The mapping analysis was conducted over a sample area of 19.25 mm \times 8.80 mm, and the value in each point is based on fitting spectra in 10 pixel \times 10 pixel areas. (c) The dual-column sample with the coordinates of the neutron diffraction scanning method shown and (d) the distribution of the (200) interplanar spacing for the sample derived from neutron diffraction. *Image courtesy of researchers/ORNL.*

Material kinetics relevant to the performance of complex engineering components span 10 orders of magnitude in the length scale, from atomic to mesoscale, as well as a middle-range size scale, situated between the microscopic and macroscopic levels. Here, analysis focuses on the behavior of a material by considering its internal microstructure—individual grains or fibers—rather than treating it as a homogenous continuum. An accurate multiscale understanding of the material system as well as the specific part with a specific manufacturing history (e.g., casting, extrusion, machining, heat treatment, surface finish) must be considered for an accurate quantification of component performance. Recent work at SNS has demonstrated the feasibility of measuring temperature evolution, elastic and plastic strains, texture, and phase fractions in real time (Plotkowski et al., 2023).

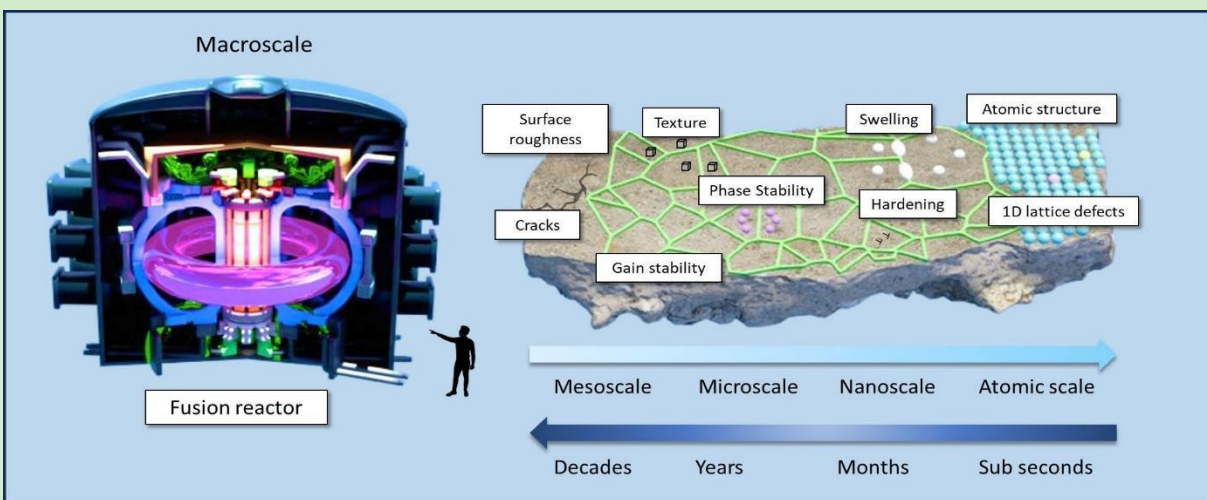
However, to understand the long-term stability of these microstructures under loading conditions, we must estimate the partitioning of alloying elements (e.g., carbon, nitrogen, and hydrogen) between phases along with the variations close to the small-scale macro defects that control the fatigue life. Extracting such elemental distributions across a practical sample volume on the order of cubic centimeters is beyond current neutron diffraction tools, which provide insufficient experimental spatial resolution at all relevant length scales.

Current sources do not provide sufficient cold neutron peak brightness and collimation required for voxelized quantitative imaging to locate damage zones that are not known a priori. New cold neutron instruments at STS will enable such studies because the target and moderator are designed to deliver the required neutron flux at the wavelength spectrum (2–15 Å) needed to realize multimodal imaging/diffraction, allowing a tensorization of the stress and strain data at the required length scales.

To date, only targeted proof-of-principle studies with limited size scales have been possible, but these are inadequate to drive advanced computer models requiring accurate operando materials data. The STS instruments will enable a detailed understanding of complex, time-dependent transformations crucial for developing advanced manufacturing processes.

Box. 5.2. Real-Time Insights into Nuclear Materials Performance at STS

STS will provide transformative capabilities for advancing the science and engineering of nuclear materials. With unprecedented peak brightness and advanced instrumentation, STS will enable researchers to observe structural materials in real time under extreme conditions such as high temperatures, mechanical stress, and radiation—conditions directly relevant to nuclear applications. The ability to perform in situ neutron diffraction and small-angle scattering simultaneously will allow for multiscale characterization, from atomic arrangements to microstructural evolution, helping to reveal how complex materials behave and degrade in demanding environments.



Example of failure-critical structural cladding component in an experimental fusion reactor. Here, material kinetics span 10 orders of magnitude in length scale, from atomic to mesoscale. Accurately predicting component performance requires a multiscale understanding of material behavior and the part’s unique manufacturing history. Image courtesy of Theresa Ahearn/ORNL.

These capabilities are particularly important for tackling long-standing challenges in nuclear materials development, such as optimizing strength and ductility without compromising other essential properties. STS will support investigations into the roles of phase boundaries, precipitate distributions, and deformation mechanisms that influence material performance. By enabling time-resolved measurements and linking structural evolution to material response, STS will generate crucial data to inform the design of next-generation structural materials for nuclear energy systems—materials that are stronger, more resilient, and capable of withstanding the harsh environments within reactors or waste containment systems.

5.2 GRAND CHALLENGE 4: MATERIALS AND PROCESSES FOR AUTONOMOUS CONSTRUCTION INNOVATION

Key Question

- How will advanced materials and processes enable autonomous, energy-efficient construction?

Advanced materials and processes will enable autonomous, energy-efficient construction by moving concrete and cementitious building processes from labor-intensive, bespoke workflows to robotic AM with formulations that are predictable and fast-curing and that reliably bond between printed layers. Today's printable cementitious materials are still limited by long and poorly controlled cure times, narrow processing windows (pumpability → extrudability → buildability), early-age cracking and shrinkage, and uncertain interlayer bonding—because the key hydration reactions, transport processes, and buried interfaces evolve rapidly inside dense, aggregate-filled materials that are difficult to probe directly. STS provides a critically important measurement backbone to break this bottleneck: high-brightness, cold, pulsed neutrons can penetrate realistic specimens and, because of their sensitivity to water and hydrogen-bearing species, STS will enable time-resolved tracking of hydration, moisture redistribution, pore formation, and interface development across nanometer-to-millimeter scales, with measurements fast enough (15 Hz) to capture transient printing states and early-age curing in situ. By combining neutron imaging/tomography with diffraction and scattering, multimodal STS instruments will link evolving microstructure and phase composition to deformation, interlayer integrity, and damage under realistic construction environments, producing decision-grade datasets that can train AI models and support closed-loop control of mix design and printing parameters—reducing energy waste, material overuse, and rework while enabling new high-performance, low-carbon construction methods.

The U.S. construction industry's current reliance on outdated, resource-intensive methods contributes significantly to the nation's energy consumption through inefficiency. Leveraging robotics and AM, combined with advances in chemistry and soft matter science, will enable a new epoch for the built environment that no longer depends on current construction methods such as cement casts. Concrete's high strength, flowability during construction, and history dating back to the Roman Empire have led to tens of gigatons being used annually, requiring more than 4 Gt of cement powder (the glue in concrete) to be manufactured each year (IEA, 2018; IEA, 2024). The global usage of concrete, on a volume basis, is second only to society's need for water, demanding massive resource and energy requirements. Innovation in manufacturing is central to the future of construction materials, where efforts will focus on AM and high-performance systems (Moini et al., 2018; Monteiro et al., 2017). Transforming how we build and what we build with will significantly influence energy dependence.

The use of advanced cements, concrete AM, and robotic construction will revolutionize the construction process and the entire built environment, both on-planet and off-planet. However, the construction process needs a paradigm shift, considering that the current standard remains dominated by manual labor, with each building being constructed by hand. These inefficiencies have generated significant economic costs, including workplace accidents, leading to elevated prices for infrastructure and housing. Autonomous robotic construction is evolving in various forms, although two main areas are currently being investigated. Robotic construction pertains to the erection of structural systems from existing building blocks (e.g., masonry units, truss members). Concrete AM constitutes the most revolutionary advance and is hybridized with the concrete former to yield the most powerful modality. For example, shotcrete (spray-deposited concrete) deposition around robotically erected reinforcing steel (rebar) allows for the fully autonomous construction of reinforced concrete structures. These examples show what is possible with significant effort and a small set of concrete mixtures.

Advancing this capability to many different forms of buildings and using a wide variety of readily available stock materials (resources currently not utilized) will require significant and dynamic development of materials and processes for which the cold neutron instruments at STS will be well-suited. Current facility capabilities are limited because the dynamic range available for experiments is not broad enough to simultaneously measure the length scales of interest (from atomic to micrometer resolution) during an in situ additive process.

For advanced manufacturing technologies like additive manufacturing STS will allow for the real-time capture of these processes, offering valuable insights that will drive material innovation, enhance product reliability, and reduce costs. These advancements will aid in the development of complex components for industries such as consumer products, automotive systems, large-scale energy infrastructure, and new construction materials like 3D printed cement. As illustrated in Figure 11, neutron scattering can be used to monitor internal strain in materials like 3D printed cement, showcasing how STS will eliminate the need for costly, labor-intensive casting methods while supporting the creation of high-performance components that align with DOE's mission to advance energy dominance, strengthen advanced manufacturing capabilities, and maintain U.S. economic competitiveness

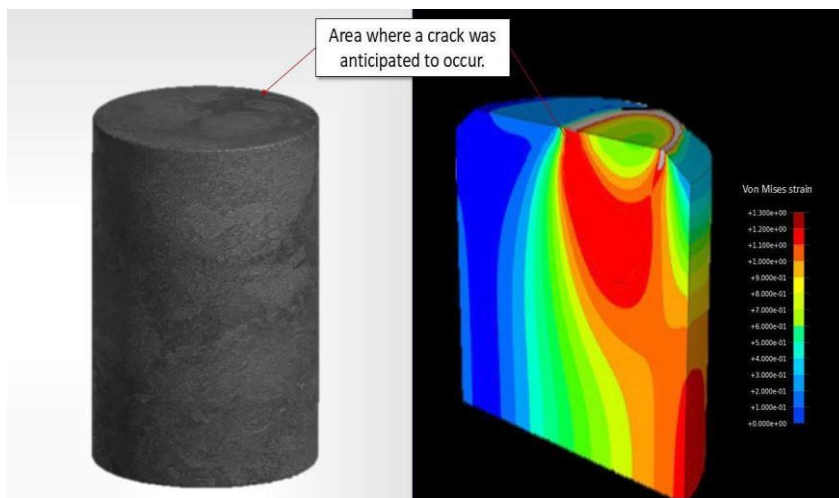


Figure 11. Neutron scattering: stress distribution and crack prediction in a cement sample. This conceptual figure illustrates how neutron scattering could be used to evaluate internal strain in a cement sample. It draws on techniques such as neutron and synchrotron X-ray tomography, destructive testing, and Bragg-edge neutron imaging to represent how a fatigue crack might be characterized. *Image courtesy of Theresa Ahearn, ORNL.*

6. SECURING U.S. RESOURCES THROUGH ADVANCED CHEMISTRY

Chemistry underpins the nation's energy security, yet key processes in catalytic and advanced energy applications remain poorly understood at the atomic level under true operando conditions. Advanced synchrotron light sources have enabled progress in studying catalytic surfaces and electronic structures under operational conditions, but they face fundamental limitations in probing hydrogen dynamics, isotope-specific behavior, and buried interfaces, especially under high-pressure, high-temperature, and chemically reactive environments essential for transformative energy research. By contrast, neutron scattering provides penetrating, nondestructive, isotope-sensitive insights into hydrogen and light elements, deep within materials, enabling critical measurements under realistic, harsh conditions that are extremely demanding to access at light sources. Building on these advantages, STS will provide up to 10 times the cold neutron brightness of current sources, broader bandwidth, and millisecond to subsecond time resolution, enabling operando studies of catalytic systems and functional materials under realistic conditions that are beyond the reach of existing neutron and light sources.

In particular, STS will address fundamental questions in catalysis, energy storage, and separations that cannot be effectively tackled with FTS, including tracking proton and ion transport in reactive environments with sufficient time resolution, quantifying reaction intermediates and hydrogen bonding in catalytic cycles with small sample mass, and observing structure and dynamics changes in advanced electrochemistry systems and porous membranes under operando conditions. These insights are essential to advancing low-energy nitrogen fixation, CO₂ capture and conversion, resilient battery chemistries,

hydrogen storage materials, critical mineral separations, advanced membrane technologies, and catalyst development for sustainable fuels—areas that demand the small sample, real-time, operando capabilities STS uniquely provides. Overall, STS will provide the precise, real-time measurements needed to design advanced catalysts and materials that are essential for U.S. energy security, decarbonization, and critical materials independence.

Impact of STS on Advanced Chemistry Research

STS will bring unique capabilities needed by the U.S. chemistry community to rapidly advance our understanding of chemical systems and drive the development of new materials and processes for securing U.S. resources.

The high brightness of STS will allow design of instruments that will allow in situ and operando experiments to be undertaken at a scientifically relevant timescale. The high brightness enables pulse-by-pulse determination of structural evolution and catalytic function, a capability that is not achievable even with FTS. High brightness also enables structural studies of microgram quantities of single crystals and powders, including from recovered phases of materials that are prepared in very small quantities using high-pressure presses and other synthetic approaches that cannot readily be scaled up or are needed for fast prototyping and materials development.

The high brightness and broad bandwidth of STS allow development of new multimodal instrument concepts that will collect data across a very broad range of length and time scales. Equipped with suitable sample environments, the instruments will be capable of isolating the composition, nature, location, and behavior of key hydrogen, lithium, carbon, nitrogen, and phosphorus atoms as well as other light element-containing species as they function and interact within engineered systems such as fuel cells, batteries, and chemical reactors as well as natural systems such as subsurface geological formations and exoplanet interiors.

Such capabilities are possible at advanced light sources; however, some key limitations exist regarding the compatibility of certain sample environments. For example, light source studies of in situ chemical reactors require the use of high-energy X-rays for penetration, limiting the applicability of certain spectroscopies. Neutron scattering in general is an advantageous way to probe the structure of materials that contain light elements. This technique, coupled with STS instruments, provides a compelling scientific case for studies of chemistry in operando conditions, enabling experiments to be conducted that are not possible at other facilities.

Neutrons are unmatched in determining the physical and chemical state of hydrogen: they are exceptionally sensitive to hydrogen and other light atoms even amidst heavier elements, and they enable studies where isotopic labeling is used to isolate a feature of interest. This sensitivity is essential to chemistry and energy grand challenges involving porous solids and membranes for separations, cathodes, anodes, and electrolytes for energy storage and electrochemical synthesis. X-rays are not a compelling probe for scientific studies where hydrogen is important; STS provides a transformative capability to leverage the properties of neutron in operando studies of chemical process where hydrogen plays a role, providing experimental capabilities that are not currently available.

6.1 GRAND CHALLENGE 5: UNLOCKING THE FUNDAMENTAL MECHANISMS GOVERNING THERMO- AND ELECTROCATALYSIS

Key Questions

- What are the underlying atomic and molecular mechanisms that govern catalytic transformations, and how can these insights enable the design of more efficient and resilient catalytic systems?

- How can we kinetically steer competitive solid–electrolyte interphase (SEI)-forming reactions to rationally design a catalytic interface in situ? What are the elementary reaction steps and their rates for the formation of individual SEI components?
- How do catalysts restructure under operating conditions? How do these changes in bulk and surface catalyst structure relate to catalyst performance? What are the relevant timescales for these reactions?

The cold neutron brightness of STS allows for instruments that will be able to tackle these catalysis and interphase questions by enabling truly operando, pulse-by-pulse measurements of catalyst structure and dynamics across atomic to mesoscale length scales at scientifically relevant rates, leveraging intense cold-neutron pulses at 15 Hz (every ~60 ms) with time resolution that can reach the millisecond regime for kinetic studies. This capability directly targets the central barriers in thermo- and electrocatalysis: transient active-site restructuring, hydrogen location and motion, short-lived intermediates, buried interfaces, and fluctuating solvation layers that control selectivity, degradation, and performance under realistic conditions. Because neutrons are highly penetrating and uniquely sensitive to hydrogen and other light elements (with isotope labeling to isolate specific species), STS can quantify how catalysts evolve inside real reaction vessels without perturbing reaction kinetics and can resolve both the structure (bulk and surface) and the dynamics needed to infer elementary steps and rates. For electrochemical systems, this same operando advantage is decisive for SEI science: SEI layers are performance-critical yet change when removed from operating conditions, so advancing from empirical formulation to predictive interface design requires in situ observation of SEI formation dynamics and competitive pathways.

Catalysis remains one of the most pressing and complex scientific frontiers in energy science, driving research to quantify how catalysts accelerate chemical reactions under realistic operating conditions, and from atomic-scale active sites to mesoscale reactor environments. The STS neutron scattering capabilities will, for first time, enable simultaneous characterization of the structure and dynamics of catalysts – and ability to probe reactivity- across multiple length and time scales. This world-unique capability will drive predictive design and delivery of efficient and optimized catalytic systems.

Catalysis is crucial to addressing the nation’s energy challenges and plays a vital role in many areas of the chemical and petrochemical industries. However, the fundamental mechanisms driving catalytic transformations under realistic conditions are still not fully understood. This knowledge gap has far-reaching implications for industrial processes, such as the Haber–Bosch process, which, although energy-intensive, is essential for producing fertilizers that help feed society. Understanding the atomic and molecular mechanisms of catalysis, particularly for electrochemical nitrogen reduction, is critical to developing more efficient solutions.

Advanced catalysis research requires time-resolved and multimodal characterization capabilities to study catalytic mechanisms in real time (Figure 12). Techniques such as X-ray scattering provide excellent opportunities for in situ studies. Neutrons studies provide complimentary data because neutrons are highly penetrating can be used to perform in situ studies in realistic high-pressure, high-temperature reaction vessels without interacting with the electronic subsystem or altering chemical reaction kinetics.

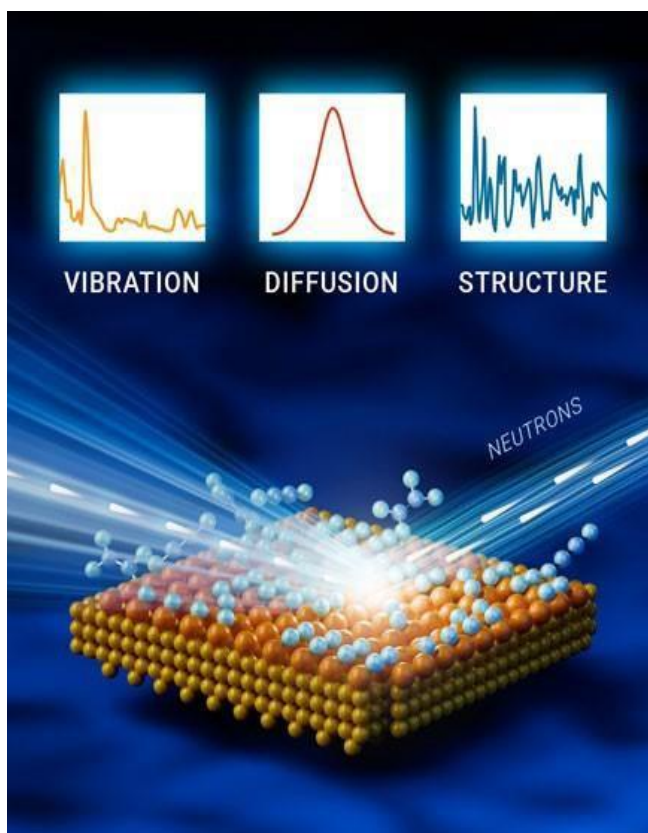


Figure 12. Neutrons reveal the dynamics of materials, showcasing vibration, diffusion, and structural properties important for catalysis. *Image refurbished and enhanced by Phoenix Pleasant. Image courtesy of the American Chemical Society.*

The ability to leverage isotope labeling with neutrons provides a powerful pathway to disentangle the contributions of specific atomic species within complex catalytic structures, allowing researchers to pinpoint how different components evolve and interact during operation. Importantly, neutron interactions do not affect chemical reactions, providing a benign probe with which to observe chemical reactions. Important for catalysis investigations is the rate at which catalysis happens: often approximately one reaction per second per active site for inorganic catalysts important for industrial processing. Although myriad details can influence catalytic rates, the one reaction per second benchmark serves as a key parameter for effective operando measurement of catalytic processes. STS will uniquely enable investigation of catalysts and catalyst reactions operando at 15 Hz because its novel high brightness neutron moderators effectively solve the brightness limitation of existing facilities. STS will deliver intense, cold neutron pulses approximately every 60 μ s. This capability will allow researchers to observe critical changes in catalysts and measure the structure and dynamics for every STS pulse, providing a unique neutron science capability not achievable elsewhere. For certain experimental modalities, the STS pulse can be further subdivided to improve available time resolution for kinetic studies. Neutrons and X-rays can provide complementary windows into catalytic processes. X-rays excel at probing electronic states, oxidation dynamics, and the structure of heavy elements with high spatial resolution. When combined with advanced X-ray techniques, neutron scattering provides an integrated view of structure, dynamics, and electronic processes capabilities essential to overcoming the grand challenges in thermal- and electrocatalysis.

STS will provide transformational capabilities to tackle grand challenges in thermo- and electrocatalysis. These grand challenges revolve around controlling complexity: predicting dynamic evolution of catalyst

structures, selective steering of multi-pathway networks, and designing active environments that extend beyond a single binding site. Meeting these challenges requires atomic-to-mesoscale, real-time insights into structure and dynamics as well as a high-fidelity view of the energy landscape of chemical reactions. STS will provide a unique suite of experimental capabilities not achievable elsewhere that will tackle these challenges and enable U.S. researchers to study the structure and dynamics of catalysts materials in realistic operating conditions, in real time with up to 8 μ s resolution, directly addressing the grand challenges outlined in a recent DOE-BES basic research needs report.¹

STS will deliver transformational capabilities for thermo- and electrocatalysis by enabling operando measurements of catalyst structure and dynamics across atomic to mesoscale length scales. Many of the most important catalytic processes—fuel production, CO₂ conversion, ammonia synthesis, biomass upgrading, water splitting, fuel cells, CO₂ reduction, and nitrogen fixation—remain limited by poor selectivity, slow kinetics, degradation, and incomplete mechanistic understanding under realistic conditions. The central challenge is controlling complexity: transient active-site restructuring, hydrogen location and motion, short-lived intermediates, buried interfaces, fluctuating solvation layers, and dynamic charge-transfer states that govern performance.

An example of how neutrons can contribute to unlocking these mechanisms involves the study of proton transfer processes within pyridoxal-5'-phosphate-dependent enzymes, which are responsible for a wide range of catalytic biochemical reactions. Neutron scattering at STS will enable precise tracking of hydrogen atom positions in enzyme active sites during different stages of catalysis, offering a detailed understanding of how proton transfer is facilitated. This approach not only contributes to better understanding of enzyme-specific catalytic transformations but also extends to industrial catalysis, such as that in energy-intensive processes. The integrated capabilities at STS—spanning neutron diffraction, inelastic scattering, and quasielastic scattering, combined with world-leading neutron brightness—will allow researchers to resolve transient intermediates, hydrogen dynamics, and reaction pathways with unparalleled precision.

Among the pressing global challenges in catalysis, the chemical reduction of dinitrogen (N₂) to ammonia (NH₃) (Figure 13) stands out as an innovative application where STS can make a groundbreaking impact. This six-electron/six-proton reduction process is one of the most challenging and important chemical transformations (Chalkley et al., 2020). The global dependence on ammonia for agriculture underscores the urgency of addressing its energy-intensive and carbon-heavy synthesis. Primarily produced via the Haber–Bosch process, NH₃ accounts for approximately 2% of global energy consumption. Modern NH₃ production requires 29.7 million BTUs of net energy per ton of nitrogen (Kongshaug 1998; Sutton et al., 2013). This energy-intensive process necessitates breakthroughs in nitrogen fixation and catalytic NH₃ synthesis methods (Ahmed et al., 2024; Chalkley et al., 2020; Weber et al., 2024; Yu et al., 2023; Z. Zhang et al., 2024). STS is uniquely poised to address this challenge through its revolutionary neutron scattering capabilities, providing insights that cannot be achieved using existing technologies.

¹ Basic Research Needs for Catalysis Science TO TRANSFORM ENERGY TECHNOLOGIES Report from the U.S. Department of Energy, Office of Basic Energy Sciences Workshop May 8–10, 2017, in Gaithersburg, Maryland

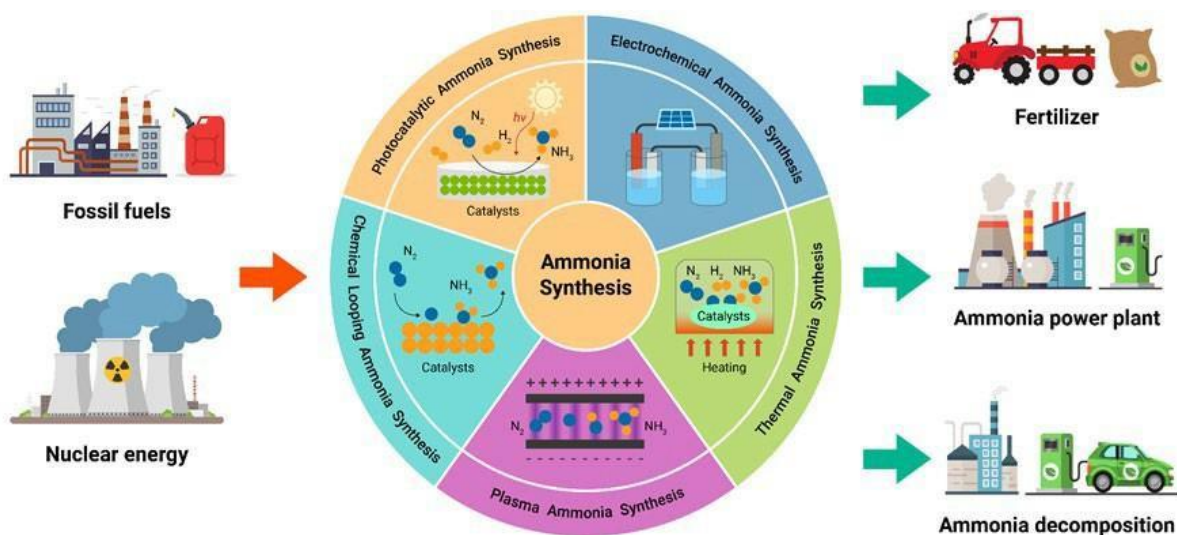


Figure 13. Schematic of in situ views of catalytic reactions. The image shows key intermediates and pathways in ammonia synthesis. *Image courtesy of Phoenix Pleasant/ORNL.*

SEI layers are performance-critical in electrochemical systems—from batteries to electrocatalytic N_2 -to- NH_3 —because they control transport, selectivity, and stability at reactive interfaces. The SEI can tune reactant activity and product selectivity by regulating species transport through the interphase while simultaneously protecting highly reactive components (e.g., lithium metal) yet maintaining ionic/electronic conductivity. Despite their importance, SEIs are difficult to design rationally because they form via coupled reactions between reactive materials and can change dramatically when removed from operating conditions, limiting the value of ex situ measurements. Advancing from empirical electrolyte formulation to predictive interphase design requires operando insight into SEI formation dynamics. STS will enable transformative progress in these areas that will generalize beyond electrocatalysis to thermo- and photocatalysis, and it will help close the gap between modeling and reality: first-principles methods capture early events over picoseconds and nanometers, whereas practical devices evolve over seconds to hours and micrometers. The grand challenge is establishing validated multiscale frameworks, anchored by real-time operando data, that connect quantum reactions to interphase growth and long-term performance.

A collaboration between Stanford University and ORNL has employed time-resolved neutron reflectometry at SNS to probe in situ processes involved in the lithium-mediated electrochemical reduction of N_2 to NH_3 (Blair et al., 2022; Blair et al., 2023; Niemann et al., 2024). Electrochemical catalysis offers a promising route for NH_3 production by enabling the process to occur under ambient conditions, thereby eliminating the high energy requirements of traditional Haber–Bosch methods. Promising next-generation NH_3 electrocatalysis systems often contain light elements such as hydrogen, lithium, nitrogen, and oxygen, which cannot be as easily tracked using X-ray scattering techniques, such as X-ray absorption spectroscopy (XAS), as they can with neutron scattering techniques. Such techniques at STS, such as reflectometry and INS, will be highly sensitive to both bulk and surface structural changes, particularly regarding the evolution of interphases between catalysis films and gas/liquid reactants. Despite recent success in probing these interface reactions using the LIQREF instrument at FTS, great challenges (e.g., time resolution) persist due to its limited brightness and narrow bandwidth. Achieving subsecond resolution requires at least twice the bandwidth and an order of magnitude increase in neutron brightness—parameters that cannot be optimized simultaneously at FTS but will be possible at STS. As such, STS is expected to be transformational for advancing this critical field.

6.2 GRAND CHALLENGE 6: ADVANCING CHEMICAL SCIENCE FOR A RESILIENT ENERGY FUTURE

Key Question

- How can breakthroughs in materials and processes enable the transition to high-efficiency energy systems and deliver energy resilience?

Breakthroughs in materials and processes are essential for enabling the transition to high-efficiency energy systems and developing energy dominance. With STS, the U.S. science community can help address critical challenges in the domestic energy sector by enhancing the efficiency and durability of solar cells, developing resilient materials for hydrogen generation, designing nuclear materials capable of withstanding extreme environments, and tackling battery degradation and material sourcing. Additionally, many advanced materials, such as those used in energy devices or solar cells, exhibit magnetic properties that can significantly influence their efficiency and stability. Neutron scattering is a powerful tool for probing these magnetic behaviors, offering valuable insights into the interactions between atomic spins and the material's overall performance under real-world conditions.

The U.S. scientific and engineering communities are uniquely positioned to address this challenge by pioneering innovations, using STS to gain a deeper understanding of complex material systems, especially processes that span multiple length and time scales and that are influenced by external stimuli or occur at interfaces. By probing complex energy systems from the macro to the atomic scale (Figure 14), STS will provide unique insights into structures, dynamic behaviors, and transformations under real-world conditions. These capabilities will allow researchers to uncover the mechanisms that drive energy processes, accelerating the discovery and optimization of functioning materials for a resilient energy future. With its high flux and precision, STS will enable scientists to study fast processes, such as catalytic reactions and phase transitions, in real time, thus providing invaluable data that traditional techniques cannot.



Figure 14. Multiscale structure of a battery cell. An illustration of the different length scales that are important to the function of a battery cell. *Image courtesy of Phoenix Pleasant/ORNL.*

Furthermore, the ability to examine materials under extreme conditions, such as high pressure, voltage, current, and temperature, reveals critical insights into their behavior and longevity, which are vital for designing more robust and efficient energy systems. The combination of advanced neutron scattering techniques and real-time data acquisition will not only enhance material design but also foster the development of innovative solutions to U.S. energy challenges.

6.2.1 Advancing High-Efficiency Photovoltaics for Solar Energy Conversion

Silicon is the most common material used in commercial photovoltaic panels; however, ongoing advancements in materials science are leading to the development of more efficient and cost-effective

thin-film, organic, and hybrid perovskite solar cells to compete with traditional technologies. Neutron scattering has already advanced our understanding of the operational principles of these organic-containing materials, particularly the dynamic properties of the cations in hybrid perovskite systems, but remaining challenges, largely linked to inefficiencies, hinder their widespread adoption. Mechanistic insight into photovoltage loss remains a major hurdle: significant energy losses occur because of phase segregation and defect-induced nonradiative recombination (Li et al., 2019). Understanding the degradation of organic photovoltaics under light, heat, and environmental stress is crucial for improving the stability of the devices (Duan et al., 2023); such experiments will be possible at STS. In addition, further experimental and computational investigations, requiring the characteristics of STS, are essential to address high defect densities and to enhance long-term performance.

6.2.2 Designing Novel Materials for Future Applications Using Domestic Supply Chains

To take full advantage of new renewable energy technologies, robust energy systems are needed to balance their intermittent nature, and these systems need access to critical minerals. The lithium-ion battery chain alone, from mining through recycling, is expected to reach a value of more than \$400 billion, with 4.7 TW capacity (McKinsey and Company, 2023) by 2030. Critical materials, including lithium, cobalt, nickel, and rare earth elements, play an essential role in enabling high-performance energy systems such as lithium-ion and redox flow batteries. However, the United States faces significant challenges in securing a stable supply of these materials because of growing demand and geopolitical supply chain concentration. Addressing these issues requires breakthroughs in material discovery and recycling technologies to meet surging energy needs (DOE, 2023). While mitigating scarce materials by using abundant materials, reducing the cost of production, and developing new materials with specific functional properties are priorities for the nation, achieving these desired outcomes is limited by existing infrastructure and capabilities, even including recently constructed fourth-generation light sources.

STS provides two clear and unique advantages to address this challenge. First, STS will enable, for the first time, operando neutron investigations of chemical reactions and chemical interactions with new materials. Although operando chemistry is routine at light sources, the X-ray cross section limits sensitivity to light elements, especially hydrogen. STS will provide fundamental insight into chemical reactions and the diffusion of ions. Because neutron cross sections are highly sensitive to light elements, STS will enable experiments that are difficult to perform at light sources. The high-fidelity STS datasets from such unique experiments will enable the development of predictive models that will facilitate the realization of a designer materials pipeline. Such a pipeline will address the need for breakthroughs in material discovery, recycling technologies, and the development of energy systems that rely on abundant and cost-effective materials, motivating the pressing need to develop high-throughput and high-fidelity characterization techniques. The faster data acquisition rates at STS will be indispensable in accelerating closed-loop material discovery and optimization (Amici et al., 2022).

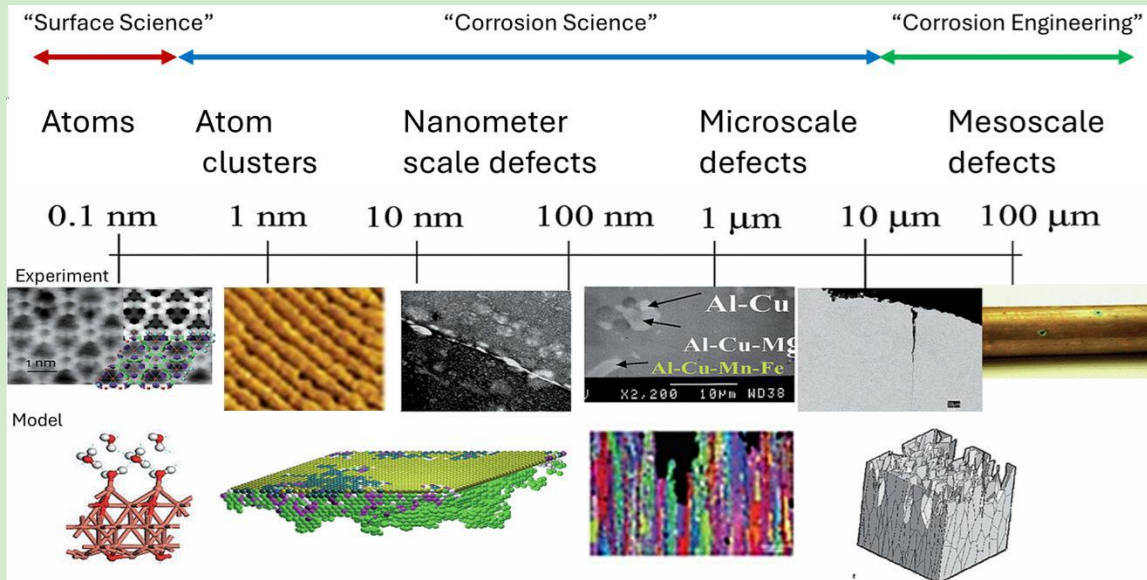
6.2.3 Advancing Understanding of Materials for Nuclear Energy and National Security

Advanced reactor designs, such as small modular reactors and molten salt reactors, are highly efficient but operate under extreme conditions, requiring advanced materials to resist corrosion, radiation damage, and high temperatures. The structure, dynamics, and reactivity of molten salts, ionic liquids, and other next-generation coolants in extreme thermal and radiolytic conditions must be investigated to optimize their design. Understanding the physics and chemistry at material interfaces is essential to control corrosion, radiolytic damage, and chemical interactions in nuclear systems (Beierschmitt et al., 2017). At the same time, the advancement of fusion reactors requires innovating plasma-facing materials to endure high neutron flux, extreme heat, and particle bombardment; this durability is crucial for the viability of fusion energy. Understanding the chemistry of heavy elements, especially actinides, from the fundamental

aspects of actinide bonding to the chemistry and stability of actinide complexes in harsh conditions, is essential for advancing next-generation nuclear reactors, developing innovative reprocessing and recycling technologies, and safeguarding society from radiological contamination. Although computational chemistry and materials science have provided another probe for complex actinide chemistry in the last decades, experimental effort remains challenging because actinides are profoundly complex compounds, and often only small quantities are available for research due to regulatory and radiation limits (Gibson and De Jong, 2018).

Box 6.1. STS Enabling Next-Generation Nuclear Energy for AI-Era Demands: The Role of the Second Target Station

AI data centers currently consume 3.5% of U.S. electricity, with projections indicating demand will surpass 9% by 2030 (Thompson and Jiang, 2024). This rapid growth far exceeds the nation’s annual energy production increase of just 1%–2%, raising urgent concerns about energy availability, reliability, and national security. Nuclear energy holds the promise to meet this challenge, but progress in advanced fission and fusion systems depends on transformative breakthroughs in understanding the materials and mechanisms that drive nuclear performance. STS is designed to address this need. With a uniquely narrow pulse structure and record-setting brightness of cold neutrons, STS will offer the precision, sensitivity, and speed required to unlock foundational discoveries in nuclear materials science and chemistry.



Multiscale visualization of corrosion, from atomic to mesoscale, using experimental and modeling.
Courtesy ORNL Researchers.

Materials in next-generation reactors—whether fuels, claddings, coolants, or structural components—undergo complex, multiscale transformations during operation. Corrosion, for instance, initiates with atomic-level redox reactions and evolves through ion migration and defect formation, ultimately producing structural damage that is visible on macroscopic scales (Quan et al., 2022). Current neutron sources lack sufficient brightness and bandwidth to allow installation of instruments that can capture these dynamics in a single experiment. STS will remove this limitation. Its advanced suite of multimodal instruments will integrate wide-angle and small-angle neutron scattering techniques to enable seamless spatial measurements from atomic to mesoscale, covering nanometers to hundreds of nanometers in real time. Coupled with the high brightness of long-wavelength neutrons, STS will provide unmatched temporal resolution for observing materials under operationally relevant conditions such as high temperature, pressure, and radiation fields. This capability is critical for studying actinides and other heavy elements central to next-generation reactor designs, which are often available only in microgram to milligram quantities and exhibit highly localized, dynamic behavior beyond the reach of current facilities. STS will overcome these barriers by combining ultrabright neutron beams with innovative sample handling, including noncontact containment methods such as acoustic levitation, and rapid data acquisition matched to evolving material states. Enabling real-time, multiscale experiments will accelerate the development of durable reactor materials, improve predictive modeling and validation, and shorten the path from discovery to reactor deployment.

7. SOFT MATTER AND POLYMERS

Soft matter materials—including polymers, colloids, liquid crystals, foams, gels, and biological macromolecules—play decisive roles in modern manufacturing, energy production, and biomedical processes. Their hierarchical structures and dynamic behaviors offer versatile frameworks for designing next-generation devices and systems.

STS will provide transformative experimental capabilities to quantify the structure and dynamics of soft materials in real time, providing US researchers with world-leading experimental capabilities that will unlock understanding of multiscale complex system behaviors that are currently considered intractable. STS will enable high-fidelity, real-time, subsecond measurements that uncover the free energy landscape in soft materials during kinetic processes and will enable researchers to understand formation pathways and create designer soft materials to address US grand challenges in energy security health and biotechnology.

Soft matter research employs a wide range of characterization tools, including microscopy, spectroscopy, and scattering methods. Among these, neutron scattering provides uniquely powerful insights and stands as a fundamental pillar of modern soft matter research.

STS will be essential for understanding how these materials work across multiple length scales in real-world conditions. Gaining the advantage of this fundamental knowledge will advance U.S. leadership in emerging energy technologies and materials innovation. These advancements will provide economic growth in manufacturing new consumer products ranging from lighter, stronger, and more versatile plastics to healthier foods without chemical additives. Soft materials and products are composed of many-component blends with large proportions of amorphous, light element, organic compounds. Many techniques, including synchrotron light source methods, are employed in characterizing soft materials, but only neutrons can directly determine what a polymer looks like and how it moves in a soft material.

Impact of STS on Soft Matter and Polymers

Understanding the hierarchical structure and dynamic evolution of soft materials is essential to drive breakthroughs in technology and innovation. Gaining this understanding requires a facility with unprecedented spatial and temporal resolution. STS, with higher neutron brightness, wide Q -range, and event-mode data collection, is uniquely positioned to address these challenges.

The signature capability of STS will be to enable simultaneous investigation of multiple length and time scales, enabling the operando study of hierarchical² materials in action as they form, flow, or shear. STS's multiscale capability would thus directly address a critical gap in soft matter research: connecting the hierarchy of structure to material function. The capability is derived from the key parameters of the STS source—world-leading cold neutron brightness and optimized bandwidth—the unique benefits of neutron scattering for soft matter systems, light element sensitivity, and non-perturbative, non-damaging interactions with matter. These parameters enable installation of instruments at STS that can capture structural and dynamic information over decades of length and time scales and accelerate understanding of multiscale complexity which is a fundamental scientific grand challenge.

² For example, a polymer nanocomposite has local polymer chain conformations (nanometer scale), dispersed filler particles (tens of nanometers), and often micrometer-scale phase-separated domains. Time scales range from fast polymer segmental motions to cluster rearrangements. Observing all requires multiple techniques, such as SANS, wide-angle diffraction, and spectroscopic methods with fine energy resolution for soft dynamics.

Many of the most pressing technological advances, ranging from sustainable materials to advanced manufacturing to energy storage and biomedical systems, depend on controlling structures and dynamics that span multiple length and time scales. Soft matter systems embody this challenge: their behavior emerges from a delicate interplay of weak intermolecular interactions, mesoscale organization, and macroscopic performance. The fundamental science of energy landscapes drives material properties and is at the core of understanding soft matter systems. Neutron scattering is a unique analytical tool for this endeavor. Understanding and ultimately controlling the free energy landscape will enable development of technologies, devices, and products that will shape societies and communities worldwide.

The free energy landscape describes the multitude of accessible configurations a system can adopt, as well as the barriers and pathways between them. STS instrumentation will provide U.S. researchers unique insights to probe energy landscapes and deliver new scientific insights into soft matter:

- **Morphology and conformation:** Understanding how polymer chains arrange, fold, and interact under different conditions is central to predicting functional outcomes such as elasticity, permeability, or conductivity.
- **Bonding and interactions interplay:** Stable covalent bonds, dynamic covalent bonds, hydrogen bonds, and many other molecular and supramolecular interactions collectively define the pathways across the free energy landscape. Mapping how these interactions compete or cooperate is essential for predictive control of self-assembly and formulation.
- **Out-of-equilibrium dynamics:** Many functional materials—such as printed polymers, thin films, or biomaterials—are created under nonequilibrium conditions (e.g., drying, shear, flow). The processing pathway defines the final structure and properties, so probing these transitions in real time is vital.
- **Enabling predictive design:** By mapping how molecules and polymers sequence and bond, and to define a navigable free energy landscape, STS will support predictive models of materials design.

Developing fundamental scientific understanding in these areas will enable microscopic control of macroscopic function. For example, guiding nanoparticle assembly into architectures during polymer matrix glass transition and solidification defines the mechanical and transport properties of the final polymer nanocomposite, just as controlling ion transport landscapes dictates the performance of solid polymer electrolytes.

The ability to probe and understand free energy landscapes is central to advancing soft materials science. STS's unique combination of neutron source parameters will create transformative capabilities. First, STS will provide world leading neutron brightness and optimized wavelength bandwidth. STS will deliver beams with 10× brightness of cold neutrons with 4× broader wavelength bandwidth compared with FTS, thus enabling the study of larger structures in soft matter systems, critical for understanding collective assembly and diffusive processes in multiscale hierarchical systems. STS will also enable real-time, in situ observation of out-of-equilibrium phenomena. The 15 Hz pulse structure and high brightness beams of STS will allow time-resolved studies that capture dynamical changes as they happen. With this capability, researchers will be able to make “movies” of transient phenomena and watch how free energy landscapes evolve during processing or function.

The STS source characteristics create the hallmark capability of STS: the ability to probe multiple length scales and timescales simultaneously pulse by pulse in operando and during kinetic processes, capturing high-fidelity time-resolved data of structures, transients, and out-of-equilibrium phenomena. This capability will be transformative for soft matter discovery and control.

STS will provide a step-change in real-time, operando neutron characterization of materials as they transform during processing, capturing structure and dynamics across multiple length scales in a single measurement. This is currently not possible in the U.S. because existing neutron sources lack three combined capabilities: wide simultaneous Q -range, high dQ/Q resolution at medium to high Q , and high brightness.

Polymer AM (3D printing) is a good example of an applied research area where STS enables something uniquely valuable: direct measurement of individual polymer-chain conformations and entanglements in complex, hydrogen-rich mixtures using isotopic (deuterium) labeling. Synchrotron small- and wide-angle X-ray scattering can access broad Q and high flux to provide valuable complimentary information, isolating signals from specific light-element components in mixtures using neutron scattering. Isotopic substitution is a direct probe that can directly measure molecular entanglement without radiation damage. STS will be the ideal facility for tracking flow, entanglement, relaxation, diffusion, and layer bonding during AM as the process unfolds—not just in the finished part.

STS's brightness, TOF/event-mode data, and 15 Hz repetition rate extend accessible time scales, allow smaller/weaker samples, and broaden the simultaneously measurable length/energy ranges, enabling repeated, parameter-swept experiments and ultimately autonomous experiment steering from real-time feedback. The outcome is faster discovery and improved manufacturing reliability in polymers/soft matter, with downstream contributions to energy, biomedical materials, and advanced manufacturing, thereby strengthening U.S. competitiveness.

7.1 GRAND CHALLENGE 7: UNDERSTANDING DYNAMICS IN NONEQUILIBRIUM SYSTEMS

Key Question

- What molecular mechanisms, such as ion transfer and phase transitions, drive dynamic and transient phenomena in soft materials?

The performance of soft materials—particularly in polymer electrolytes, flow-induced crystallization, and adaptive gels—depends critically on their dynamics under nonequilibrium conditions. Processes spanning molecular motions to large-scale structural transitions drive applications in energy generation, manufacturing, and health care. For instance, efficient ion transport in polymer electrolytes directly enhances energy output in batteries, and shear-induced transitions govern the mechanical properties of advanced plastics in 3D printing or coating technologies. However, understanding the molecular mechanisms, such as ion transport and phase transitions, that drive these dynamic and transient phenomena remains limited. This gap in knowledge hinders the ability to capture these processes in real time, a challenge that STS can address directly by enabling neutron scattering measurements of structure and dynamics at 15 Hz on a pulse-by-pulse basis. Data from STS instruments will improve understanding of these dynamic processes and of nonequilibrium systems, leading to the development of high-performance materials and systems without compromising lifespan.

Understanding and addressing the grand challenge of time- and energy-dependent processes in soft matter will lead to significant advancements in science and technology (Hemminger et al., 2015). By unraveling the intricate connections between molecular motions, transient phenomena, and macroscopic behaviors, researchers can design materials with unprecedented adaptability, functionality, and efficiency. These insights have transformative implications for energy dominance, health care, and manufacturing, driving innovation across a broad range of fields.

7.1.1 Revolutionizing Adaptive Polymer Manufacturing and Processing

Studying the flow and deformation of polymers during shear and extrusion will enhance manufacturing processes, such as 3D printing and deposition of advanced coatings (Gantenbein et al., 2018; Rowland et al., 2008; Varol et al., 2017; Zhang et al., 2024). Insights into nonequilibrium dynamics gained through STS time-resolved neutron scattering data will enable the design of materials with superior mechanical and functional properties, driving manufacturing advancements and creating more efficient and cost-effective production processes for cutting-edge technologies. Flow-induced molecular orientation and dynamic relaxation into entangled states are crucial for layer bonding and the resulting durable manufactured polymer components. The findings from STS instruments will facilitate the development of adaptive polymer materials capable of self-organization during processing, leading to smarter and more advanced manufacturing practices that optimize material performance, reduce waste, and minimize energy consumption.

7.1.2 Enabling Advanced Energy and Conversion

Real-time observation of ion transport, polymer relaxation, and molecular dynamics under nonequilibrium conditions is critical for advancing energy and conversion materials (Do et al., 2013; Sun et al., 2015; Yoshimune et al., 2024). Today, neutron scattering plays a significant role in providing fundamental understanding of these complex multicomponent soft materials by revealing both structure and dynamics at the molecular and nanoscale level (Zhan et al., 2018). This capability is facilitated chiefly by tunable neutron contrast, which enables highlighting specific molecules and structural features, combined with the advantageous simultaneous match of neutron wavelength and energy with molecular length and time scales. Further advancement in these areas is currently not possible due to the limited neutron flux at existing facilities. To overcome this limitation requires brighter neutron beams that deliver more neutrons in small volumes, enabling time-dependent studies of molecular processes as well as spatially resolved studies, such as mapping molecular orientation across interfaces during polymer AM.

Time-resolved neutron scattering at STS, only possible because of the high brightness and large wavelength bandwidth, will provide unique capabilities to resolve transient phenomena, such as solid–electrolyte interface formation in batteries and dynamic processes in conjugated polymers, across femtosecond to nanosecond timescales. STS will enable the decoupling of backbone and side-chain dynamics, revealing how molecular structures govern charge transport, thermal stability, and optoelectronic performance. For instance, current studies have linked side-chain motion to charge transport efficiency in polythiophenes, and we have uncovered slow collective dynamics related to π – π stacking (Guilbert et al., 2019). Operando studies are essential for elucidating material response at the molecular level during device operation. These transient and nonequilibrium processes are difficult to study with high fidelity when they are removed from their operando context.

7.1.3 Innovating in Biomedical Applications

Understanding the molecular-level dynamic responses of hydrogels and polymers under physiological conditions will lead to breakthroughs in controlled drug delivery, self-healing materials, and tissue engineering (Scotti et al., 2016; Zhao et al., 2023). Neutron and X-ray user facilities have contributed significant advances in understanding the details of structure in complex biomedical materials such as lipid nanoparticles for drug delivery. Further progress in the field requires observing in situ and in real time how these molecular assemblies respond to and interact with their target locations, such as during lipid membrane fusion. Such studies require neutron contrast variation for highlighting specific molecules and nanoscale structures. They also require good Q resolution for resolving sharp scattering signals. These capabilities are available at FTS (Qian et al., 2022; Qian and Rai 2018), but current neutron

scattering capabilities have neither sufficient beam brightness nor simultaneous Q -range to observe the full picture of a lipid nanoparticle fusing with a cellular membrane.

Better, more tailored, polymeric and lipid-assembly-based materials will offer new and improved biomedical applications for targeted drug delivery and artificial replacement tissues alike. Neutron and X-ray facilities have significantly contributed to the development of such materials, but STS will change the game by enabling studies of such materials in their realistic dynamic context as encountered in applications. STS neutron scattering data will be used to reveal how polymer relaxation and molecular-scale interactions govern the response and adaptability of these materials.

These advancements will improve patient outcomes and reduce health care costs by allowing more effective and durable biomedical interventions. Moreover, the ability to tailor material behavior in response to specific stimuli will unlock opportunities for developing personalized medical devices and therapies, significantly enhancing the precision and effectiveness of health care technologies.

7.1.4 Unveiling Mechanisms in Nonequilibrium Complex Fluids

Capturing structural and dynamic response in glassy or jammed systems under stress will provide fundamental insights into yielding and flow behavior, with broad commercial applications from aerospace and automotive lubrication to food science. Complex fluids are materials that exhibit properties between those of simple liquids and solids, often possessing a hierarchical structure and including components like polymers, colloids, and gels.

Current facilities cannot cover the dynamic and spatial range required to investigate complex fluids; therefore, progress in this area is limited. Overcoming these limitations requires new capabilities. Neutron scattering at STS will enable real-time studies of these complex systems, providing fundamental data to optimize materials for industrial applications such as lubricants and protective coatings (Liu et al., 2020; Meng et al., 2022; Schmid et al., 2023).

Synchrotron light sources, even when providing wide length scales, are limited by lack of contrast variation options required to discern information from specific, individual molecules in these complex systems, and they cause radiation damage effects. The unparalleled cold neutron brightness of STS enables experiments in real time, allowing investigation of operando processes for glassy or jammed systems and providing data that will be used to enhance the performance and reliability of materials critical for infrastructure and industry. Furthermore, understanding these mechanisms will inform the development of advanced composites and materials with tailored stress-response properties, such as shock resistance of lubricants and flexible body armor, enabling new capabilities in construction, transportation, and energy.

7.2 GRAND CHALLENGE 8: MASTERING HIERARCHICAL ASSEMBLY AND MULTISCALE DESIGN

Key Question

- How will real-time characterization of emerging hierarchical structures advance design of adaptive materials for energy dominance, health care, and advanced manufacturing?

The ability to understand and control hierarchical assembly is a fundamental challenge in materials science because structural organization at one scale directly influences functionality at larger scales. Many advanced materials, from high-performance polymers to biological tissues, derive their properties from complex architectures spanning multiple length scales. Unlike simple crystalline solids, these materials lack long-range order and instead rely on dynamic, multicomponent assemblies where

molecular-level interactions dictate macroscopic behavior. For example, rubber tires achieve mechanical resilience through a combination of polymer chemistry, crosslinking density, and the dispersion of reinforcing fillers. Similarly, polymer-based electrolytes and electrode composites in energy systems depend on a delicate balance between nanoscale ion transport channels and mesoscale structural stability to optimize conductivity and longevity. Despite their importance, these multiscale interactions remain difficult to study because of limitations in current experimental techniques. A key question is how real-time characterization of emerging hierarchical structures can advance the design of adaptive materials for energy dominance, health care, and advanced manufacturing.

Existing characterization methods—such as UV–visible, infrared, and Raman spectroscopy—are excellent for identifying local chemistry and bonding, but they do not directly resolve nanoscale organization or follow time-dependent structural rearrangements as materials evolve. Likewise, electron microscopy and X-ray scattering can deliver high-quality structural snapshots at selected length scales, yet they generally cannot track hierarchical transitions seamlessly across the coupled nano- to mesoscale landscape or under realistic, time-dependent processing conditions. Synchrotron light sources provide a set of options for contrast variation for certain systems. However, with light elements or where hydrogen is important, isolating the behavior of specific components within the complex remains challenging, and for some experiments radiation damage can distort the results. Without a high brightness source of cold neutrons, there is a persistent characterization gap where directly probing how multiscale architectures form, transform, and relax in real time is challenging or impossible.

Addressing this challenge requires experimental tools capable of spanning atomic to microscale structures while capturing dynamic changes as they occur. STS will offer an unprecedented window into hierarchical material formation by enabling simultaneous, real-time observation across length scales ranging from angstroms to hundreds of nanometers. The high-brightness neutron source, combined with a broad wavelength band and large detector coverage, will allow researchers to track structural evolution continuously rather than relying on disconnected snapshots (Figure 15). Neutrons will allow researchers to observe the behavior and interaction of individual, labeled molecules in the context of evolving, complex systems. This capability is crucial as the complexity of synthetic materials begins to approach that of biological systems. By providing a comprehensive view of hierarchical structuring, STS will enable a more predictive approach to materials design, allowing precise control over molecular topology, chemical sequence, and emergent properties.

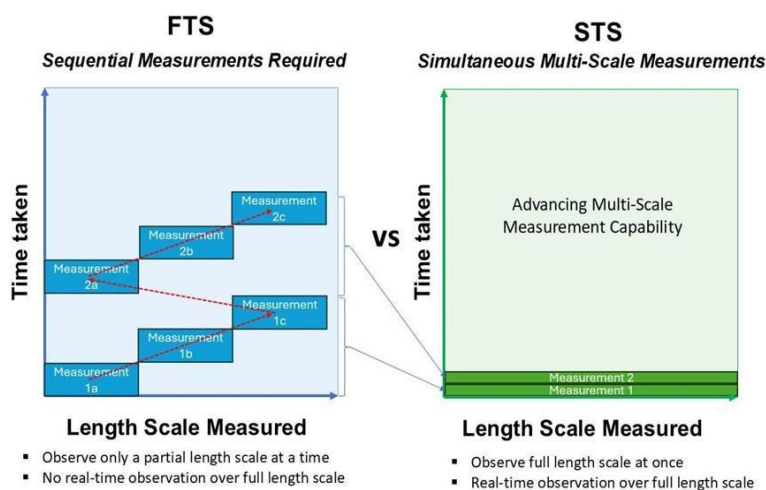


Figure 15. Length scale measured. Diagram showing how measurements across wide length and time scales are performed at STS compared with FTS or HFIR. STS instruments can observe the full range of length scales simultaneously, whereas existing instruments at FTS or HFIR can observe only partial ranges, leaving structural knowledge gaps that STS instruments will eliminate. *Image courtesy: Changwoo Do/ORNL.*

7.2.1 Advancing Nature-Inspired and Adaptive Systems

Nature offers a compelling blueprint for hierarchical material design, where functionality emerges from self-assembly processes across multiple length scales. Biological materials, such as protein structures and natural adhesives, demonstrate how molecular interactions govern macroscopic properties, enabling exceptional mechanical resilience, controlled molecular transport, and self-healing behavior. Replicating these principles in synthetic materials could yield breakthroughs in energy, biomedicine, and functional soft matter, but realizing these novel materials requires a deeper understanding of the structural transitions that drive self-assembly.

One example is the design of protein-inspired block copolymers, which mimic the precision of biomolecular structures. Researchers have explored sequence-defined polymer architectures that integrate synthetic block copolymer self-assembly with biological design principles. Helical self-assembly, for instance, spans multiple length scales, but although molecular-level organization is well understood, its influence on larger-scale structural and material properties remains unclear (Castelletto et al., 2020; Murnen et al., 2010). Previous studies have shown that achiral, partially charged block copolypeptoids can spontaneously form right-handed helices with monodisperse diameters. However, current techniques cannot fully resolve how molecular-scale stacking leads to emergent chirality. STS, with its broad length-scale coverage and high brightness, will allow researchers to directly probe lamellar stacking within helices and reveal the symmetry-breaking mechanisms responsible for homochirality. Furthermore, the high neutron flux will permit real-time subsecond observation of early-stage molecular assembly, providing unprecedented insights into intermediate structures that dictate final morphology.

Another example is complex polymer coacervates, which undergo liquid–liquid phase separation driven by electrostatic attractions between oppositely charged polyelectrolytes. Inspired by biological systems such as mussel adhesives and squid beak structures, coacervates hold promise for applications in medical adhesives, drug delivery, and 3D bioprinting (Wang et al., 2024). However, a fundamental understanding of polyelectrolyte behavior in solution remains elusive, particularly given the broad range of hierarchical structures involved. In aqueous environments with salts, ion condensation effects introduce strong correlations across multiple length scales, significantly influencing structure and dynamics. Current experimental techniques struggle to capture these interactions across wide length scales simultaneously.

STS will overcome these limitations by providing unprecedented access to simultaneous wide Q -range measurements, enabling detailed structural characterization from molecular to mesoscopic scales within single experiments. Instruments such as SANS, wide-angle neutron scattering, and neutron reflectometry will allow researchers to systematically investigate how molecular topology, chemical sequence, and intermolecular forces influence coacervate stability. By decoding these long-standing mysteries at multiple length scales, STS will facilitate the predictive design of coacervate-based materials with tailored hierarchical properties, accelerating their use in biomedical and industrial applications.

By providing real-time, multiscale insights into hierarchical material assembly, STS will transform the design and application of nature-inspired materials. These advances will lead to tailored biomimetic structures, enabling breakthroughs in adaptive energy materials, self-healing polymers, and biofunctional architectures. The ability to bridge the molecular-to-macroscopic divide will finally allow researchers to apply nature’s design strategies with unprecedented precision, unlocking new frontiers in soft matter physics, polymer science, and engineered materials.

7.2.2 Mastering Nature-Inspired Material Design with STS

Biological systems excel at creating complex, hierarchical materials with precision and adaptability, providing a blueprint for designing advanced materials with tailored properties. However, replicating

these multiscale processes in synthetic systems remains a challenge because vast spatial and temporal scales are involved: from angstroms to micrometers and from fractions of a second to days. Current techniques lack the capability to simultaneously capture the full spectrum of these processes, limiting the ability to understand and control self-assembly mechanisms essential to material functionality.

STS will allow researchers to simultaneously probe atomistic details and mesoscale structures with subsecond time resolution—an unprecedented capability not possible at current neutron sources or near-term European facilities. By enabling real-time measurements across broad length and time scales, STS bridges the critical knowledge gap between molecular interactions and macroscopic properties, paving the way for materials that mimic the precision, adaptability, and functionality of natural systems.

Similarly, polymer coacervates inspired by marine organisms, such as mussel adhesives and sandcastle worm glue, hold immense promise for applications including 3D bioprinting, tissue scaffolding, and advanced adhesives. As illustrated in Figure 16, STS will enable time-resolved studies of coacervation kinetics, revealing the influence of ion condensation, molecular topology, and electrostatic correlations on their dynamic assembly and mechanical properties. These insights will allow for predictive design of high-performance coacervates with finely tuned interactions and complex 3D architectures engineered for targeted real-world applications. STS will also unlock the ability to observe how dynamic soft material systems evolve under external stimuli such as temperature gradients, shear forces, or solvent environments. Such observations include in situ and operando studies of polymers and biological materials undergoing phase transitions, aggregation, or crystallization—conditions that are central to processing and function. These measurements, made possible by STS’s small beam size and high brightness, will inform the design of new adaptive, recyclable, and self-healing materials.

By providing unparalleled real-time, multiscale characterization capabilities, STS will empower researchers to harness nature’s principles to create materials with extraordinary precision, responsiveness, and efficiency. These breakthroughs will accelerate innovation across health care and energy, helping to solve some of the most pressing technological and societal challenges.

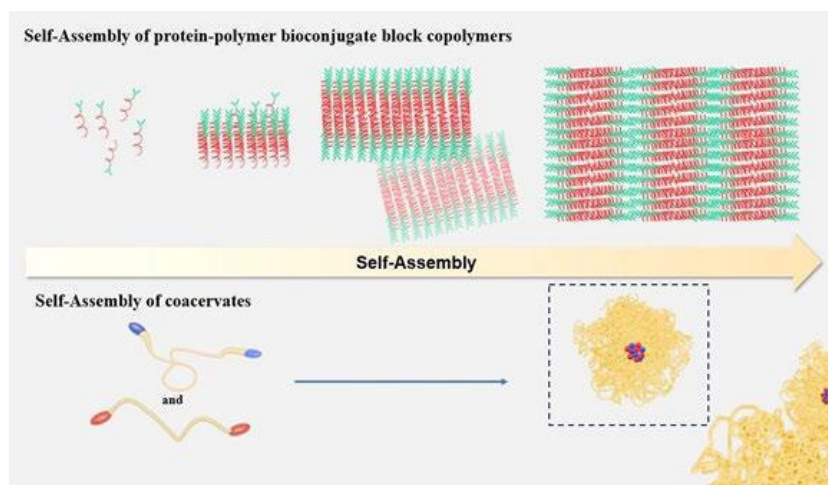


Figure 16. Two nature-inspired self-assembly processes. (top) Protein polymer bioconjugate block copolymers form nanostructured assemblies. (bottom) Charged polyelectrolyte triblocks condense into dynamic coacervate micelles and gels (Srivastava et al., 2017). *Image courtesy Theresa Ahearn/ORNL.*

8. BIOLOGICAL SYSTEMS: REVOLUTIONIZING FOUNDATIONAL BIOMEDICAL RESEARCH AND BIOMATERIALS

STS has immense potential to resolve critical scientific challenges in health care, agriculture, and bioinspired concepts across society. The astonishing progress of experimental structural biology and AI in recent years has enabled the development of structure prediction tools such as AlphaFold. Yet, as powerful as these methods are, they fail to precisely locate hydrogen atoms within biomolecules, predict the structure of complex biomolecular assemblies, or describe the motions of biomolecules that govern their functions. For example, hydrogen atoms constitute nearly half of the atoms in biomolecules and play crucial roles in hydrogen bonding, proton transport, enzyme catalysis, and drug binding. Unlike X-ray crystallography and electron microscopy, neutron scattering is a unique method to resolve hydrogen positions needed to quantify these critical biomolecular functions.

Impact of STS on Biological Systems

Historically, neutron scattering has fallen short of its promise in this area due to limitations in neutron flux and intensity, requiring extended data acquisition times and limited resolution. Biological samples are precious and are available in very small volumes, at narrowly defined experimental conditions, and over short periods of stability. These technical restrictions prevent the comprehensive study of complex biomolecular interactions, how these structures change on biological timescales, and the dynamic biological processes in the unique time and length scales available to inelastic neutron scattering. Our inability to systematically execute advanced biophysical studies on real biological samples hinders progress in areas such as enzyme kinetics, synthetic biology, drug discovery, bioenergy, and biomaterial design.

STS provides a solution to these obstacles by delivering significant increases to neutron flux (data acquisition times), neutron intensity (precious samples), and spatial and temporal resolution for dynamics (neutron wavelength optimization). These advances will enable unprecedented insights into hydrogen positions, catalysis, the dynamic structures of complex biomolecular assemblies, membrane biophysics, and molecular motions. This revolutionary capability will address critical scientific gaps, driving breakthroughs across synthetic biology, bioenergy, agriculture/ecological systems, and health care. STS is not simply an upgrade in neutron capability—it is a necessary transformation that aligns with the next era of structural biology, enabling data that cannot be accessed through any other technique.

8.1 GRAND CHALLENGE 9: ENGINEERING THE PRINCIPLES OF LIFE

Key Question

- How can predictive understanding of the designs and mechanisms underpinning the principles of life enable advances in areas such as biocatalysis, biopharmaceuticals, biopreparedness, and energy conversion?

A revolution in structural biology has occurred with the introduction of AI/ML structure prediction algorithms. AlphaFold (Jumper et al., 2021) and similar methods provide sequence-to-structure predictions with remarkable speed and accuracy. However, critical information on hydrogen atom positions is missing from all these predictions. As AI and ML continue to accelerate structure prediction, STS provides the experimental counterpart to validate, refine, and expand these models with real hydrogen-resolved structural data. Hydrogen atoms play pivotal roles in drug binding and enzymatic catalysis, where proteins perform chemically valuable reactions. Understanding how hydrogen bonds contribute to the specificity, stability, and kinetics of enzymatic reactions; deciphering how protons move through complex protein systems; recognizing the role of structured water in stabilizing protein

complexes, ribosomes, or viral capsids; and observing subtle hydrogen bond rearrangements in allosteric or conformational changes are all critical to understanding the central mechanisms of biological function.

Current AI models are built upon hundreds of thousands of protein structures deposited in the Protein Data Bank. Neutron protein crystallography precisely provides the information needed to complete these structural predictions. However, this information is underrepresented in the Protein Data Bank because of the low number of available neutron structures. Protein crystals of high-value therapeutic targets can typically be grown only to small sizes, well below 0.1 mm³, which current neutron sources lack the brightness to study. This shortcoming has prevented the study of many important proteins, including protein kinases that regulate phosphorylation—a critical post-translational modification involved in cell growth, differentiation, and apoptosis. Dysregulated kinase activity often leads to cancer and inflammatory diseases.

Neutron scattering is uniquely capable of probing the structure and motions associated with enzymes that orchestrate electron transfer chains without perturbing the redox state. X-rays and electrons commonly used to characterize these structures can photoexcite redox cofactors. Consequently, many of the structures in the Protein Data Bank represent photoreduced states that have been altered by X-rays or electron characterization methods, rather than natural states (Carugo and Carugo, 2005). STS will enable measurement of out-of-equilibrium processes associated with local redox chemistry and longer-range conformational dynamics, both of which are necessary for understanding the control of electron transfer. With its unprecedented combination of brightness and time resolution, STS will allow researchers to directly observe redox-driven conformational changes as they occur, providing new insights into how enzymes regulate electron flow in biological systems.

Due to the high brightness and increased bandwidth available at STS, its neutron protein crystallography instruments will achieve 20-fold performance gains relative to instruments at FTS. Additional gains of 10- to 100-fold can be achieved by polarizing the incident neutron beam while deploying advanced sample environments for dynamic nuclear polarization of hydrogen atoms within the protein crystal (Pierce et al., 2020). Thus, by combining the high brightness of STS and dynamic nuclear polarization of the sample, performance gains of up to 1,000-fold over current neutron protein crystallography instruments are possible, allowing the study of high-value therapeutic targets that have thus far been impossible to study with neutron diffraction. This new set of capabilities will revolutionize the field, expanding structural knowledge from neutrons and providing vital information that can be used to develop more effective drugs with fewer side effects while improving the understanding of enzymatic catalysis and how proteins perform chemically valuable reactions.

The wavelength characteristics of STS will greatly enhance studies of cell membranes and membrane proteins. Understanding lipid structure, dynamics, and how lipids modulate protein function in membranes is critical for biological processes ranging from fermentation to complex signal transduction and vesicle fusion in human cells. The long wavelength design of STS permits the development of new small-angle scattering instruments and neutron spin echo spectrometers with greater flux at the relevant scattering wavevectors for lipid studies.

Enzymes are dynamic and catalyze reactions along pathways that involve transient intermediates and conformational changes on timescales spanning picoseconds to milliseconds or more. STS will enable comprehensive descriptions of macromolecular function by revealing sequence–structure–dynamics relationships via inelastic scattering methods, time-resolved SANS, and diffraction. Dissecting dynamic mechanisms requires combining tailored sample environments and computational techniques to provide unprecedented mechanistic views of enzyme chemistry. The high brightness and increased bandwidth available at STS will allow researchers to determine several static structures of freeze-trapped intermediates in days rather than months, opening the door to kinetic neutron crystallography. Time-

resolved SANS allows investigators to follow the structural change in proteins, protein assemblies, and other biomacromolecules over the course of milliseconds to seconds. This capability will allow exploration of dynamic structures in both the ordered and disordered (flexible) regions of proteins and complexes.

8.1.1 Bioenergy and the Circular Bioeconomy

The isotopic sensitivity of neutrons combined with the high hydrogen content of biomass and biomembranes make neutron scattering techniques a powerful suite of tools to study the structure and organization of the plant cell wall and how it changes due to genetic modifications or chemical and biochemical deconstruction. Starch-based fuels and biomaterials are a key part of the American transportation fuel landscape: in 2023, approximately 13.7 billion gallons of ethanol were blended into U.S. gasoline (U.S. Energy Information Administration 2024). Active research is ongoing to employ lignocellulosic feedstocks for transportation fuels and other bioproducts.

Lignocellulosic feedstocks do not generally compete with food crops and are available at lower cost with less intensive cultivation costs. Additional processing is needed to deconstruct this class of biomass.

Neutrons can resolve the structure and organization of the plant cell wall and how it changes due to genetic modifications or chemical and biochemical deconstruction. The increased bandwidth at STS will allow, for the first time, simultaneous characterization of lignocellulosic materials at wide spatial scales, from nanometers to micrometers, during deconstruction. STS will also enable researchers to track structural changes in living plants to gain insight into the evolving structure of cell walls during growth. This capability has the potential to guide the genetic engineering of plants with desirable properties for technological applications. Observing structural changes in biomass in real time during deconstruction is crucial for determining process conditions for deconstruction of biomass. Currently, the time resolution of these measurements is limited to minutes (Shah et al., 2019); however, with the higher brightness and increased bandwidth at STS, structural changes could be resolved on subsecond timescales. This information is vital for designing plants that are optimized for biofuel and bioproduct production.

Enzymes also play key roles in bioenergy production; for example, they break down lignocellulosic biomass for biofuel generation. The advanced neutron diffraction capabilities at STS will uncover how hydrogen bonds, water localization, and proton transport influence enzyme stability and efficiency, enabling the design of more robust biocatalysts for renewable energy applications. Fermentation is another key step in biofuel and bioproduct production. Maximizing biofuel fermentation titer, yield, and productivity are crucial considerations to control cost because higher concentrations of the product from fermentation reduce the energy demand of subsequent separation steps. Cellular membranes in fermentative microorganisms are the target of solvent toxicity. So, to maximize titer, fermentative microbes must be made more tolerant of solvent and toxic byproducts. SANS, again leveraging the optimized neutron wavelengths of STS, and neutron contrast-matching techniques can resolve the complex interactions of enzymes, solvents, membrane lipids, and lignocellulosic biomass.

8.1.2 Agricultural Processes

The future circular bioeconomy and food security require continuous development within the agricultural sector. Neutrons, with their sensitivity to light elements and ability to nondestructively probe living materials—combined with the new capabilities of STS—will facilitate new experiments that are able to study the rhizosphere, where roots and soils interact. Microbial cells, such as bacteria, archaea, fungi, and viruses, do not live in isolation but communicate with each other using chemical signals. This form of cell-to-cell communication, known as quorum sensing (QS), regulates microbial populations. Within the rhizosphere, QS governs biofilm formation, a crucial part of the nitrogen fixation cycle that is vital to

agriculture. The formation of biofilms is essential for morphological differentiation and is responsible for some forms of antimicrobial resistance.

Studying cellular membranes in QS microbial colonies is believed to be a promising strategy because the membrane represents a potential target for new antibiotics. Altering the bacterial membrane could provide a method to shut down QS and its harmful consequences. Neutron scattering and isotopically labeled bacteria offer the possibility of studying bacterial membranes with nanometer resolution in QS bacterial colonies. However, bacterial membranes make up only approximately 1–2 wt % of the total bacterial colony. The increased neutron flux offered by STS will enable, for the first time, the study of QS bacterial colonies on the nanoscale to address the urgent global threat posed by antibiotic-resistant bacteria.

Another important area where neutrons can contribute is developing a multiscale understanding of water dynamics in plants and their surrounding rhizosphere (Carminati et al., 2007; Carminati et al., 2009). Increased spatial resolution, coupled with higher flux at STS, will enable a comprehensive picture of water and nutrient movement in soils, uptake by roots, and distribution throughout plants. This information from enhanced neutron imaging capabilities will help advance understanding of water-use efficiency and can inform the engineering of crop resilience.

8.2 GRAND CHALLENGE 10: UNDERSTANDING THE MOLECULAR BASIS OF HEALTH, AGING, AND WELL-BEING

Key Question

- How can neutron scattering at STS enhance understanding of biomolecular condensates, hydrogen dynamics in disease-related proteins, and the molecular basis of learning and memory, ultimately advancing drug development and personalized medicine?

Neutron techniques leverage isotopic substitution (e.g., deuterium labeling) to distinguish specific atomic interactions and hydrogen dynamics, enabling precise studies of metabolic pathways, signaling networks, and stress responses. Diseases such as Alzheimer’s and Parkinson’s involve protein misfolding and aggregation, and neutron scattering techniques can investigate hydrogen and hydration dynamics in amyloid fibrils or prion proteins, offering insights into the mechanisms underlying these pathologies.

Biomolecular condensates are membraneless cellular structures formed via phase separation to regulate biological processes such as gene regulation, stress responses, and viral capsid assembly (Guenza, 2023). Mutations in these proteins can lead to diseased states, including neurodegeneration and cancer. One example is amyotrophic lateral sclerosis, caused by mutations in fused-in sarcoma, an RNA-binding protein. Neutron scattering, with its unique capabilities for deuteration and contrast matching, offers unparalleled insights into the internal molecular network structure of condensates.

A current limitation in studying these systems using neutrons is the amount of sample required and the long measurement times, making it difficult to study their dynamic properties. The increased brightness at STS will enable kinetic and dynamic measurements that will transform the understanding of relationships between the internal structure of biomolecular condensates and their viscoelastic and other material properties, thereby enhancing understanding of their biological functions across all kingdoms of life and their roles in human disease.

Many therapeutic drugs depend on hydrogen bonding with their target proteins. Neutron studies enable accurate characterization of these interactions, providing critical data to optimize drug binding, efficacy, and selectivity, particularly for challenging targets like G protein–coupled receptors. A deep understanding of the relationship between genotype and phenotype—health versus disease—will transform personalized medicine.

Although X-ray techniques have determined nearly 190,000 structures, they do not provide direct information on hydrogen atom locations, which are essential for understanding ligand binding, protein interactions, and enzyme mechanisms. The high brightness and increased bandwidth available at STS for neutron protein crystallography instruments will result in 20-fold performance gains relative to instrumentation at FTS, with additional gains from techniques such as dynamic nuclear polarization. This capability will enable the characterization of high-value therapeutic targets that have been impossible to study with neutron diffraction, accelerating drug development.

8.2.1 Treatments for Neurological Disorders

The human brain contains more than 85 billion neurons, which form approximately 100 trillion synapses, many of which are associated with learning and memory (Herculano-Houzel, 2009). Understanding the molecular basis of learning and memory will enable effective control and modification of the brain's neural network and the prevention and treatment of neurological diseases.

Recently, artificial membranes have been used to study the molecular basis of learning and memory (Scott et al., 2022; Scott et al., 2023). When exposed to electrical stimulation similar to that occurring in the human brain, artificial membranes have been shown to form both short-term and long-term memories. The current data support the interpretation that the neuronal plasma membrane serves as a model for understanding biological memory and as a therapeutic target for brain diseases that do not respond to protein-targeted drugs. Therefore, a new class of lipophilic drugs must be developed to treat neurodegenerative diseases, including Alzheimer's and schizophrenia (Collier et al., 2025).

Presently, the static and dynamic structures that give rise to learning and memory in these model membrane systems, made from droplet interface bilayers only fractions of millimeters thick, are not well understood. Specular and off-specular neutron reflectometry is an ideal technique to study these neuronal membranes in all three dimensions with angstrom resolution. However, the signal from off-specular scattering from membrane lateral correlations and in-plane structures is extremely weak.

Consequently, off-specular neutron reflectometry is rarely used because the current suite of neutron sources does not have the requisite neutron flux to support this capability. STS, with its increased neutron flux and highly polarized neutrons, will open new possibilities in neurobiology. It will become part of a growing suite of experimental capabilities contributing to the treatment of neurological disorders, such as dementia, migraine, and epilepsy, that affect tens of millions of people worldwide.

8.2.2 Biosecurity and Biopreparedness

Biosecurity, or protecting against biological threats, has never been more critical. Neutron scattering has already contributed to developing lipid nanoparticle delivery systems for mRNA vaccines—a game changer in combating infectious diseases like COVID-19—and to understanding the structural biology of the virus's replication machinery.

Advances at STS will enable detailed structural and functional information about hydrogen-rich biothreat agents, such as toxins or pathogenic proteins, essential for designing neutralizing agents and protective strategies. Furthermore, approaches must be developed to stabilize and package vaccines, antibodies, and drugs for rapid deployment during pandemic situations. The capabilities of STS will help elucidate water interactions with proteins and other biomacromolecules, enabling optimization of hydration properties for vaccines and monoclonal antibodies to ensure stability during storage and distribution.

Additionally, increased bandwidth and faster measurement times will allow researchers to probe interactions between proteins, viruses, and cells with biomedical material surfaces, informing

interventions to prevent disease spread. Hydrogen dynamics play a key role in how pathogens survive under environmental stress. The advanced capabilities at STS have the potential to uncover these mechanisms, aiding strategies to mitigate the spread of pathogens in water, soil, and air.

STS will also allow researchers to probe hydrogen bonding networks in enzymes and membranes to learn how to improve their ability to detoxify biothreat agents or environmental contaminants resulting from biological attacks. Neutrons can also elucidate how hydrogen dynamics in enzymes contribute to resistance mechanisms.

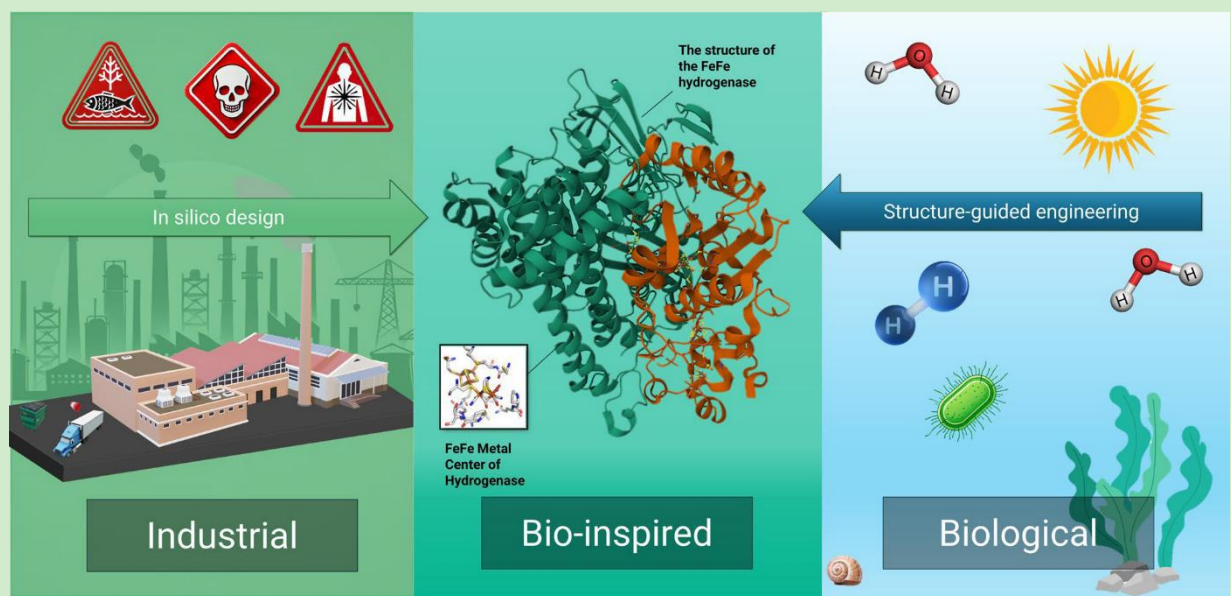
The neutron diffraction capabilities at STS will allow researchers to uncover the mechanisms of these enzymes, supporting the development of new antibiotics or resistance-modulating therapies. Overall, STS will provide unprecedented opportunities for understanding hydrogen networks from individual proteins to entire cellular systems, informing responses to pathogens and the development of systems capable of functioning in extreme or contaminated environments, aiding bioremediation and biodefense.

Box 8.1. Nature-Inspired Catalysts Will Power Our Economy

Nature uses common base metals (e.g., iron, copper, manganese) organized within transient organic scaffolds (proteins) to fix nitrogen and carbon, capture light, split water, generate hydrogen, and break down (and repurpose) complex waste streams and materials, all at ambient temperature and in aqueous solution. To translate natural processes to industrial setups, we must understand the molecular designs that enable living systems to capture, transfer, convert, and store solar/chemical energy. These investigations will inspire the development of new classes of catalysts and devices that operate under near-ambient conditions and are custom-designed and engineered to power and support an independent energy future (Sedenho et al., 2023).

We are now gaining an understanding of how metal-containing biocatalysts function in atomic detail. The key lies in uncovering how hydrogen atoms move within biological structures during these catalytic reactions, a phenomenon uniquely observable using neutron scattering techniques.

Understanding and harnessing the chemistries and design rules that enzymes use to catalyze reactions in living systems will require the rapid characterization of hundreds of enzymes as they work, in real time. With the 200-fold increase in performance that will be made available by STS and the application of neutron dynamic polarization, we will produce molecular movies of the chemical reactions catalyzed by enzymes in action. This knowledge will transform how we design new classes of industrial catalysts that are optimized to perform under ambient temperatures, pressures, and pH levels to reduce energy costs and improve more economical manufacturing processes.



Industrial, bioinspired, and biological approaches to converting substrate into product. Industrial methods often rely on harsh conditions, whereas bioinspired design and natural biological systems offer cleaner, safer, and more efficient solutions for chemical transformations. *Image courtesy Theresa Ahearn, Phoenix Pleasant, and Duncan Harryman/ORNL.*

8.2.3 From Molecules to Medicine: Exploring Biomolecular Condensates with Neutrons

Alterations in condensates are implicated in diseases ranging from neurodegeneration to cancer. Despite their significance, the complex architecture and dynamic nature of condensates challenge our

understanding, leaving fundamental questions about their structure and function unresolved. Neutron scattering, combined with deuteration, offers unparalleled opportunities to probe the internal molecular networks of condensates. Techniques such as SANS can elucidate their multiscale organization and dynamics, providing insights unavailable using other methods. However, existing neutron sources limit the resolution and scope of such studies.

STS promises a transformative leap forward. With an approximately 200-fold increase in performance, STS will enable unprecedented exploration of biomolecular condensates (Figure 17). For example, researchers will be able to capture real-time data on the kinetics of condensate formation and aging while mapping the associated changes in their hierarchical organization. Additionally, STS will help elucidate the relationships between internal network structure, viscoelastic properties, and biological functions. The enhanced capabilities of STS are poised to revolutionize the field. By deepening our understanding of the physical principles governing condensates, STS will facilitate the development of new therapeutic approaches for neurodegenerative diseases, improve strategies for enhancing plant stress tolerance, and provide insights into other critical biological systems.

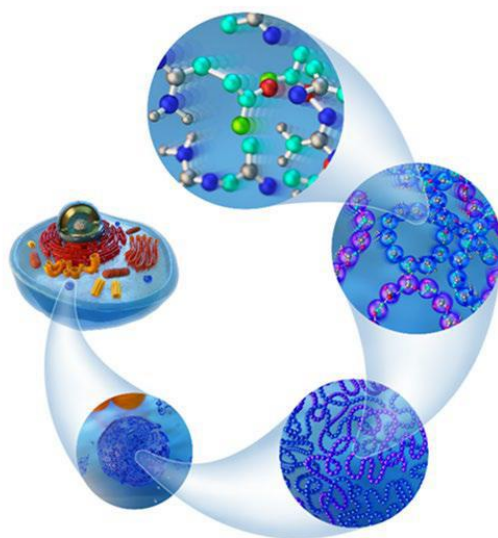


Figure 17. Schematic representation of biomolecular condensates. Showcased are their hierarchical structure and dynamic nature at different molecular scales. *Image courtesy of Phoenix Pleasant/ORNL.*

9. SUMMARY AND SUBSEQUENT STEPS

STS will be a powerful resource for energy abundance, leadership in scientific and technological innovation, and U.S. competitiveness. STS is the third component of ORNL's 3-Source Strategy and a complementary element of the nation's basic science ecosystem. Its facilities will enable technological breakthroughs critical for energy, engineering, and innovation, closing a critical characterization gap.

Accelerating the construction of STS is imperative for technological advancements in emerging fields essential to U.S. industry. Furthermore, an accelerated project timeline will result in significant cost savings.

STS will play a crucial role in addressing the grand challenges identified by the scientific community, including elucidating quantum coherence and decoherence, advancing construction and manufacturing

technologies, and enabling real-time studies of dynamic biological processes. Without STS, the United States risks losing its historic leadership in neutron science. European nations are making significant investments in facilities such as ESS, while China is rapidly expanding its neutron research infrastructure, including upgrades to the CSNS. If the United States is unable to close the characterization gap within its facilities, the nation risks experiencing irreversible technology gaps in critical fields such as quantum computing, energy materials, biotechnology, and advanced manufacturing—sectors central to global competitiveness and energy dominance.

This report describes grand challenges that STS will address, closing a key capability gap in the U.S. facility landscape. The design, prioritization, and road map for a suite of world-leading STS instruments has not yet been completed – the process or science prioritization and development of a STS instrument road map will continue with regular and transparent community engagement. Figure 18 illustrates a notional timeline for future community consultations, including key selection meetings to define and refine the initial instrument suite and key instrument capabilities, the future roadmap for STS, and, importantly, the schedule for first science at STS.

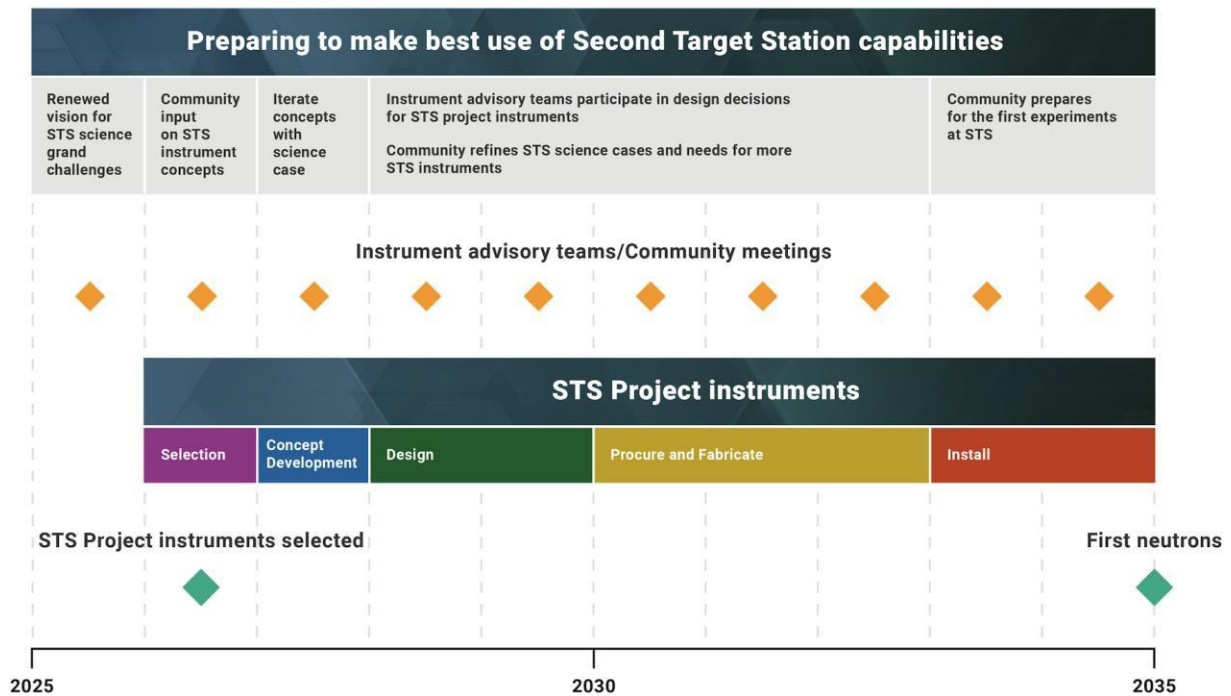


Figure 18. Notional timeline for selection of STS instruments that will be built by the STS Project, followed by design, procurement, fabrication, and installation. The timeline depends on project funding. Future instrument selection is anticipated to follow a similar process. *Image courtesy of Phoenix Pleasant/ORNL.*

10. REFERENCES

- Adams, Paul, et al. "First Experiments: New Science Opportunities at the Spallation Neutron Source Second Target Station (abridged)." Dec. 2019. <https://doi.org/10.2172/1784174>
- Ahmed, H. S., Yahya, Z., Ali khan, W., and Faraz, A. (2024). "Sustainable Pathways to Ammonia: A Comprehensive Review of Green Production Approaches." *Clean Energy*, 8(2), 60-72. <https://doi.org/10.1093/ce/zkae002>.
- Amici, J., Asinari, P., Ayerbe, E., Barboux, P., Bayle-Guillemaud, P., Behm, R. J., Berecibar, M., Berg, E., Bhowmik, A., Bodoardo, S., Castelli, I. E., Cekic-Laskovic, I., Christensen, R., Clark, S., Diehm, R., Dominko, R., Fichtner, M., Franco, A. A., Grimaud, A., Edström, K., et al. (2022). "A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+." *Advanced Energy Materials*, 12(17), 2102785. <https://doi.org/10.1002/aenm.202102785>.
- Anderson, K., DeBeer, S., Dobbins, T., Dosch, H., Epps, T., Gao, Y., Garcia, J., Huq, A., Isaacs, E., Jones, K., and Pascarelli, S. (2024). "Report on New and Upgraded National User Facilities in Basic Energy Sciences." <https://www.osti.gov/biblio/2476315>.
- Beierschmitt, K., Buchanan, M., Clark, A., Robertson, I., Britt, P., Navrotsky, A., Burns, P., Tortorelli, P., Misra, A., Wishart, J., Fenter, P., Gewirth, A., Wirth, B., Mincher, B., Szlufarska, I., Busby, J., Horton, L., Garrett, B., Vetrano, J., et al. (2017). "Basic Research Needs for Future Nuclear Energy: Report of the Basic Energy Sciences Workshop for Future Nuclear Energy, August 9-11, 2017." <https://www.osti.gov/biblio/1616270>.
- Blair, S. J., Doucet, M., Browning, J. F., Stone, K., Wang, H., Halbert, C., Avilés Acosta, J., Zamora Zeledón, J. A., Nielander, A. C., Gallo, A., and Jaramillo, T. F. (2022). "Lithium-Mediated Electrochemical Nitrogen Reduction: Tracking Electrode–Electrolyte Interfaces via Time-Resolved Neutron Reflectometry." *ACS Energy Letters*, 7(6), 1939-1946. <https://doi.org/10.1021/acsenerylett.1c02833>.
- Blair, S. J., Doucet, M., Niemann, V. A., Stone, K. H., Kreider, M. E., Browning, J. F., Halbert, C. E., Wang, H., Benedek, P., McShane, E. J., Nielander, A. C., Gallo, A., and Jaramillo, T. F. (2023). "Combined, Time-Resolved, in Situ Neutron Reflectometry and X-ray Diffraction Analysis of Dynamic SEI Formation during Electrochemical N₂ Reduction." *Energy and Environmental Science*, 16(8), 3391-3406. <https://doi.org/10.1039/D2EE03694K>.
- Castelletto, Valeria, Jani Seitsonen, Janne Ruokolainen, Cristian Piras, Rainer Cramer, Charlotte J. C. Edwards-Gayle, and Ian W. Hamley. (2023). "Peptide Nanotubes Self-Assembled from Leucine-Rich Alpha Helical Surfactant-Like Peptides." *Nanoscale Advances*, 5 (16): 1215–1224. <https://doi.org/10.1039/D3NA00129F>.
- Carminati, A., and Flühler, H. (2009). "Water Infiltration and Redistribution in Soil Aggregate Packings." *Vadose Zone Journal*, 8(1), 150-157. <https://doi.org/10.2136/vzj2008.0077>.
- Carminati, A., Kaestner, A., Hassanein, R., Ippisch, O., Vontobel, P., and Flühler, H. (2007). "Infiltration through Series of Soil Aggregates: Neutron Radiography and Modeling." *Advances in Water Resources*, 30(5), 1168-1178. <https://doi.org/10.1016/j.advwatres.2006.10.006>.
- Chalkley, M. J., Drover, M. W., and Peters, J. C. (2020). "Catalytic N₂-to-NH₃ (or -N₂H₄) Conversion by Well-Defined Molecular Coordination Complexes." *Chemical Reviews*, 120(12), 5582-5636. <https://doi.org/10.1021/acs.chemrev.9b00638>.
- Chen, Y., Cernatescu, I., Venkatesh, V., Stoica, A. D., and An, K. (2023). "On the Residual Stress Relaxation in Inconel 718 Superalloys at High Temperature by Real-Time Neutron Diffraction." *Materials and Design*, 232, 112135. <https://doi.org/10.1016/j.matdes.2023.112135>.

- Chen, Z., Andrejevic, N., Drucker, N. C., Nguyen, T., Xian, R. P., Smidt, T., Wang, Y., Ernstorfer, R., Tennant, D. A., Chan, M., and Li, M. (2021). “Machine Learning on Neutron and X-ray Scattering and Spectroscopies.” *Chemical Physics Reviews*, 2(3), 031301. <https://doi.org/10.1063/5.0049111>.
- Cheng, Y., Wu, G., Pajeroski, D. M., Stone, M. B., Savici, A. T., Li, M., and Ramirez-Cuesta, A. J. (2023). “Direct Prediction of Inelastic Neutron Scattering Spectra from the Crystal Structure.” *Machine Learning: Science and Technology*, 4(1), 015010. <https://doi.org/10.1088/2632-2153/acb315>.
- Do, C., Lunkenheimer, P., Diddens, D., Götz, M., Weiß, M., Loidl, A., Sun, X.-G., Allgaier, J., and Ohl, M. (2013). “Transport in Poly(Ethylene Oxide) Based Electrolytes: Neutron Scattering, Dielectric Spectroscopy, and Molecular Dynamics Simulations.” *Physical Review Letters*, 111(1), 018301. <https://doi.org/10.1103/PhysRevLett.111.018301>.
- DOE. (2023). U.S. Department of Energy Critical Materials Assessment. <https://www.energy.gov/sites/default/files/2023-05/2023-critical-materials-assessment.pdf>.
- Duan, L., Walter, D., Chang, N., Bullock, J., Kang, D., Phang, S. P., Weber, K., White, T., Macdonald, D., Catchpole, K., and Shen, H. (2023). “Stability challenges for the commercialization of perovskite– silicon tandem solar cells.” *Nature Reviews Materials*, 8(4), 261-281. <https://doi.org/10.1038/s41578-022-00521-1>
- Gantenbein, S., Masania, K., Woigk, W., Sesseg, J. P. W., Tervoort, T. A., and Studart, A. R. (2018). “Three-dimensional printing of hierarchical liquid-crystal-polymer structures.” *Nature*, 561(7722), 226-230. <https://doi.org/10.1038/s41586-018-0474-7>
- Gibson, J. K. and De Jong, W. A. (2018). *Experimental and theoretical approaches to actinide chemistry*. J. Wiley and Sons Ltd. <https://doi.org/10.1002/9781119115557>
- Guenza, M. (2023). Dynamics of protein droplets revealed by bridging multiple scales. *Nature*, 619(7971), 700-701. <https://doi.org/10.1038/d41586-023-02215-2>
- Guilbert, A. A. Y., Zbiri, M., Finn, P. A., Jenart, M., Fouquet, P., Cristiglio, V., Frick, B., Nelson, J., and Nielsen, C. B. (2019). “Mapping microstructural dynamics up to the nanosecond of the conjugated polymer P3HT in the solid state.” *Chemistry of Materials*, 31(23), 9635-9651. <https://doi.org/10.1021/acs.chemmater.9b02904>
- Hashimoto, T., Amino, N., Nishitsuji, S., and Takenaka, M. (2019). “Hierarchically self-organized filler particles in polymers: cascade evolution of dissipative structures to ordered structures.” *Polymer Journal*, 51(2), 109-130. <https://doi.org/10.1038/s41428-018-0147-2>
- Hemminger, J. C., Sarrao, J., Crabtree, G., Flemming, G., and Ratner, M. (2015). “Challenges at the frontiers of matter and energy: Transformative opportunities for discovery science.” <https://www.osti.gov/biblio/1283188>
- Herculano-Houzel, S. (2009). “The human brain in numbers: a linearly scaled-up primate brain.” *Frontiers in Human Neuroscience*, 3. <https://doi.org/10.3389/neuro.09.031.2009>
- IEA. (2018). “Technology Roadmap: Low-Carbon Transition in the Cement Industry.” OECD/IEA. <https://www.iea.org/reports/technology-roadmap-low-carbon-transition-in-the-cement-industry>
- IEA. (2024). *Electricity 2024*. <https://www.iea.org/reports/electricity-2024>
- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S. A. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., . . . Hassabis, D. (2021). “Highly accurate protein structure prediction with AlphaFold.” *Nature*, 596(7873), 583-589. <https://doi.org/10.1038/s41586-021-03819-2>

- Kongshaug, G. (September 28-October 1, 1998). Energy Consumption and Greenhouse Gas Emissions in Fertilizer Production International Fertilizer Association Technical Conference, Marrakech, Morocco.
- Laurell, P., Scheie, A., Dagotto, E., Tennant, D. A. (2025). “Witnessing entanglement and quantum correlations in condensed matter: A review” *Adv. Quantum Technol.* 8, 2400196. <https://doi.org/10.1002/qute.202400196>
- Li, N., Tao, S., Chen, Y., Niu, X., Onwudinanti, C. K., Hu, C., Qiu, Z., Xu, Z., Zheng, G., Wang, L., Zhang, Y., Li, L., Liu, H., Lun, Y., Hong, J., Wang, X., Liu, Y., Xie, H., Gao, Y., . . . Zhou, H. (2019). “Cation and anion immobilization through chemical bonding enhancement with fluorides for stable halide perovskite solar cells.” *Nature Energy*, 4(5), 408-415. <https://doi.org/10.1038/s41560-019-0382-6>
- Linker, T. M., Krishnamoorthy, A., Daemen, L. L., Ramirez-Cuesta, A. J., Nomura, K., Nakano, A., Cheng, Y. Q., Hicks, W. R., Kolesnikov, A. I., and Vashishta, P. D. (2024). “Neutron scattering and neural-network quantum molecular dynamics investigation of the vibrations of ammonia along the solid-to-liquid transition.” *Nature Communications*, 15(1), 3911. <https://doi.org/10.1038/s41467-024-48246-9>
- Liu, J., Lin, S., Liu, X., Qin, Z., Yang, Y., Zang, J., and Zhao, X. (2020). “Fatigue-resistant adhesion of hydrogels.” *Nature Communications*, 11(1), 1071. <https://doi.org/10.1038/s41467-020-14871-3>
- McKinsey and Company. (2023). “Battery 2030: Resilient, sustainable, and circular.” <https://doi.org/https://www.mckinsey.com/industries/automotive-and-assembly/our-insights/battery-2030-resilient-sustainable-and-circular>
- McMurtrey, M., and Messner, M. (2021). “Qualification Challenges for Additive Manufacturing in High Temperature Nuclear Applications.” ASME 2021 Pressure Vessels and Piping Conference,
- Meng, X., Qiao, Y., Do, C., Bras, W., He, C., Ke, Y., Russell, T. P., and Qiu, D. (2022). “Hysteresis-free nanoparticle-reinforced hydrogels.” *Advanced Materials*, 34(7), 2108243. <https://doi.org/https://doi.org/10.1002/adma.202108243>
- Moini, M., Olek, J., Youngblood, J. P., Magee, B., and Zavattieri, P. D. (2018). “Additive manufacturing and performance of architected cement-based materials.” *Advanced Materials*, 30(43), 1802123. <https://doi.org/https://doi.org/10.1002/adma.201802123>
- Monteiro, P. J. M., Miller, S. A., and Horvath, A. (2017). “Towards sustainable concrete.” *Nature Materials*, 16(7), 698-699. <https://doi.org/10.1038/nmat4930>
- National Academies of Sciences, Engineering and Medicine. (2024). “The current status and future direction of high-magnetic-field science and technology in the United States.” The National Academies Press. <https://doi.org/doi:10.17226/27830>
- Nickel, H., Ennis, P. J., Schubert, F., and Schuster, H. (1982). “Qualification of metallic materials for application in advanced high temperature gas-cooled reactors.” *Nuclear Technology*, 58(1), 90-106. <https://doi.org/10.13182/NT82-A32962>
- Niemann, V. A., Doucet, M., Benedek, P., Deissler, N. H., Mygind, J. B. V., Lee, S.-W., Amador, I. R., Willoughby, W., Chorkendorff, I., Nielander, A., Tarpeh, W., and Jaramillio, T. (2024). In situ neutron reflectometry reveals the interfacial microenvironment driving electrochemical ammonia synthesis. *ChemRxiv*. <https://doi.org/10.26434/chemrxiv-2024-8g61h-v2>
- Pierce, J., Cuneo, M. J., Jennings, A., Li, L., Meilleur, F., Zhao, J., and Myles, D. A. A. (2020). Chapter Eight – “Dynamic nuclear polarization enhanced neutron crystallography: Amplifying hydrogen in biological crystals.” In P. C. E. Moody (Ed.), *Methods in Enzymology* (Vol. 634, pp. 153-175). Academic Press. <https://doi.org/https://doi.org/10.1016/bs.mie.2019.11.018>

- Plotkowski, A., Saleeby, K., Fancher, C. M., Haley, J., Madireddy, G., An, K., Kannan, R., Feldhausen, T., Lee, Y., Yu, D., Leach, C., Vaughan, J., and Babu, S. S. (2023). “Operando neutron diffraction reveals mechanisms for controlled strain evolution in 3D printing.” *Nature Communications*, 14(1), 4950. <https://doi.org/10.1038/s41467-023-40456-x>
- Rowland, H. D., King, W. P., Pethica, J. B., and Cross, G. L. W. (2008). “Molecular confinement accelerates deformation of entangled polymers during squeeze flow.” *Science*, 322(5902), 720-724. <https://doi.org/doi:10.1126/science.1157945>
- Qian, S. and Rai, D. K. (2018). “Grazing-angle neutron diffraction study of the water distribution in membrane hemifusion: From the lamellar to rhombohedral phase,” *J. Phys. Chem. Lett.* 9 (19), 5778-5784. <https://doi.org/10.1021/acs.jpcllett.8b01602>
- Qian, Shuo, William Heller, Wei-Ren Chen, Andrew Christianson, Changwoo Do, Yangyang Wang, Jiao Y. Y. Lin, Thomas Huegle, Chenyang Jiang, Cristina Boone, Cameron Hart, and Van Graves. 2022. “CENTAUR: The Small- and Wide-Angle Neutron Scattering Diffractometer/Spectrometer for the Second Target Station at SNS.” *Review of Scientific Instruments* 93 (7): 075104. <https://doi.org/10.1063/5.0087625>.
- Schmid, J., Armstrong, T., Dickhardt, F. J., Iqbal, S. R., and Schutzius, T. M. (2023). “Imparting scalephobicity with rational microtexturing of soft materials.” *Science Advances*, 9(51), ead30324. <https://doi.org/doi:10.1126/sciadv.adj0324>
- Scott, H. L., Bolmatov, D., Podar, P. T., Liu, Z., Kinnun, J. J., Doughty, B., Lydic, R., Sacci, R. L., Collier, C. P., and Katsaras, J. (2022). “Evidence for long-term potentiation in phospholipid membranes.” *Proceedings of the National Academy of Sciences*, 119(50), e2212195119. <https://doi.org/doi:10.1073/pnas.2212195119>
- Scott, H. L., Bolmatov, D., Premadasa, U. I., Doughty, B., Carrillo, J.-M. Y., Sacci, R. L., Lavrentovich, M., Katsaras, J., and Collier, C. P. (2023). “Cations control lipid bilayer memcapacitance associated with long-term potentiation.” *ACS Applied Materials and Interfaces*, 15(37), 44533-44540. <https://doi.org/10.1021/acsami.3c09056>
- Scotti, A., Gasser, U., Herman, E. S., Pelaez-Fernandez, M., Han, J., Menzel, A., Lyon, L. A., and Fernández-Nieves, A. (2016). “The role of ions in the self-healing behavior of soft particle suspensions.” *Proceedings of the National Academy of Sciences*, 113(20), 5576-5581. <https://doi.org/doi:10.1073/pnas.1516011113>
- Sedenho, G. C., Colombo, R. N. P., and Crespilho, F. N. (2023). “Insights from enzymatic catalysis: A path towards bioinspired high-performance electrocatalysts.” *ChemCatChem*, 15(15), e202300491. <https://doi.org/https://doi.org/10.1002/cctc.202300491>
- Shah, R., Huang, S., Pingali, S. V., Sawada, D., Pu, Y., Rodriguez, M., Jr., Ragauskas, A. J., Kim, S. H., Evans, B. R., Davison, B. H., and O’Neill, H. (2019). “Hemicellulose–cellulose composites reveal differences in cellulose organization after dilute acid pretreatment.” *Biomacromolecules*, 20(2), 893-903. <https://doi.org/10.1021/acs.biomac.8b01511>
- Sham, T.-L. and Natesan, K. (2017). Code Qualification Plan for an Advanced Austenitic Stainless Steel, Alloy 709, for Sodium Fast Reactor Structural Application International Conference on Fast Reactors and Related Fuel Cycles: Next Generation Nuclear Systems for Sustainable Development (FR17), Yekaterinburg (Russian Federation). https://inis.iaea.org/search/search.aspx?orig_q=RN:49085870
- Scheie, A. O., Ghioldi, E. A., Xing, J., et al., (2024). “Proximate spin liquid and fractionalization in the triangular antiferromagnet KYbSe₂.” *Nature Physics* 20, 74. <https://doi.org/10.1038/s41567-023-02259-1>.

- Scheie, A., Laurell, P., Simeth, W., Dagotto, E., Tennant, D. A. (2025). “Tutorial: Extracting entanglement signatures from neutron spectroscopy.” *Materials Today Quantum* 5, 100020. <https://doi.org/10.1016/j.mtquan.2024.100020>
- Srivastava, S., Andreev, M., Levi, A. E., Goldfeld, D. J., Mao, J., Heller, W. T., Prabhu, V. M., de Pablo, J. J., and Tirrell, M. V. (2017). Gel phase formation in dilute triblock copolyelectrolyte complexes. *Nature Communications*, 8(1), 14131. <https://doi.org/10.1038/ncomms14131>
- Sun, C. N., Zawodzinski, T. A., Tenhaeff, W. E., Ren, F., Keum, J. K., Bi, S., Li, D., Ahn, S. K., Hong, K., Rondinone, A. J., Carrillo, J. M. Y., Do, C., Sumpter, B. G., and Chen, J. (2015). “Nanostructure enhanced ionic transport in fullerene reinforced solid polymer electrolytes.” *Physical Chemistry Chemical Physics*, 17(12), 8266-8275. <https://doi.org/10.1039/c4cp05583g>
- Sutton, M. A., Reis, S., Riddick, S. N., Dragosits, U., Nemitz, E., Theobald, M. R., Tang, Y. S., Braban, C. F., Vieno, M., Dore, A. J., Mitchell, R. F., Wanless, S., Daunt, F., Fowler, D., Blackall, T. D., Milford, C., Flechard, C. R., Loubet, B., Massad, R., . . . de Vries, W. (2013). “Towards a climate-dependent paradigm of ammonia emission and deposition.” *Philosophical Transactions of the Royal Society B: Biological Sciences*, 368(1621), 20130166. <https://doi.org/doi:10.1098/rstb.2013.0166>
- Tang, S., Venkatakrisnan, S. V., Chowdhury, M. S. N., Yang, D., Gober, M., Nelson, G. J., Cekanova, M., Biris, A. S., Buzzard, G. T., Bouman, C. A., Skorpenske, H. D., and Bilheux, H. Z. (2024). “A machine learning decision criterion for reducing scan time for hyperspectral neutron computed tomography systems.” *Scientific Reports*, 14(1), 15171. <https://doi.org/10.1038/s41598-024-63931-x>
- Thompson, W., and Jiang, B. (2024). “Artificial Intelligence is hungry for power, Barclays 3 point perspective.” <https://www.ib.barclays/our-insights/3-point-perspective/AI-power-energy-demand.html>
- Varol, H. S., Meng, F., Hosseinkhani, B., Malm, C., Bonn, D., Bonn, M., Zaccone, A., and Parekh, S. H. (2017). Nanoparticle amount, and not size, determines chain alignment and nonlinear hardening in polymer nanocomposites. *Proceedings of the National Academy of Sciences of the United States of America*, 114(16), E3170-E3177. <https://doi.org/10.1073/pnas.1617069114>
- Walck, M., Abergel, R., Uberuaga, B., Wharry, J., Laverne, J., Gleason-Holbrook, A., Couet, A., Glezakou, V., Crockett, T., Horton, L., McLean, G., Schwartz, A., Vetrano, J., Wilk, P., Severs, L., Beatty, A., Woods, B., Brooks, R., Heinrich, E., and Ozcan, G. (2024). *Basic Energy Sciences Roundtable: Foundational Science to Accelerate Nuclear Energy Innovation*. <https://www.osti.gov/biblio/2481526>
- Walsh, A. C., Nienow, S., Merker, J., Decker, E., Strack, C., Salem, M., Marting, G., and Shaw, B. (2024). “Assessment of the retrospective and prospective economic impacts of investments in U.S. neutron research sources and facilities from 1960 to 2030. RTI International.
- Wang, H., Zhuang, H., Tang, W., Zhu, J., Zhu, W., and Jiang, L. (2024). Coacervate-pore complexes for selective molecular transport and dynamic reconfiguration. *Nature Communications*, 15(1), Article 10069. <https://doi.org/10.1038/s41467-024-54510-9>
- Weber, J. E., McMillion, N. D., Hegg, A. S., Wertz, A. E., Aliahmadi, M., Mercado, B. Q., Crabtree, R. H., Shafaat, H. S., Miller, A. J. M., and Holland, P. L. (2024). “Isocyanide ligation enables electrochemical ammonia formation in a synthetic cycle for N₂ Fixation.” *Journal of the American Chemical Society*, 146(49), 33595-33607. <https://doi.org/10.1021/jacs.4c11187>
- Yoshimune, W., Higuchi, Y., Song, F., Hibi, S., Matsumoto, Y., Hayashida, H., Nozaki, H., Shinohara, T., and Kato, S. (2024). “Neutron imaging for automotive polymer electrolyte fuel cells during rapid cold starts.” *Physical Chemistry Chemical Physics*, 26(47), 29466-29474. <https://doi.org/10.1039/d4cp03646h>

- Yu, X., Cheng, Y., Li, Y., Polo-Garzon, F., Liu, J., Mamontov, E., Li, M., Lennon, D., Parker, S. F., Ramirez-Cuesta, A. J., and Wu, Z. (2023). "Neutron scattering studies of heterogeneous catalysis." *Chemical Reviews*, 123(13), 8638-8700. <https://doi.org/10.1021/acs.chemrev.3c00101>
- Zhan, P., Zhang, W., Jacobs, I. E., Nisson, D. M., Xie, R., Weissen, A. R., Colby, R. H., Moulé, A. J., Milner, S. T., Maranas, J. K., and Gomez, E. D. (2018). Side chain length affects backbone dynamics in poly(3-alkylthiophene)s. *Journal of Polymer Science, Part B: Polymer Physics*, 56(17), 1193-1202. <https://doi.org/10.1002/polb.24637>
- Zhang, C., Hua, W., Mitchell, K., Raymond, L., Delzendehrooy, F., Wen, L., Do, C., Chen, J., Yang, Y., Linke, G., Zhang, Z., Krishnan, M. A., Kuss, M., Coulter, R., Bandala, E., Liao, Y., Duan, B., Zhao, D., Chai, G., and Jin, Y. (2024). "Multiscale embedded printing of engineered human tissue and organ equivalents." *Proceedings of the National Academy of Sciences of the United States of America*, 121(9), Article e2313464121. <https://doi.org/10.1073/pnas.2313464121>
- Zhang, Z., Zhang, H., Jiang, H., and Li, L. (2024). "Green ammonia: revolutionizing sustainable energy for a carbon-free future." *Journal of Materials Chemistry A*, 12(48), 33334-33361. <https://doi.org/10.1039/D4TA07339H>
- Zhao, Y., Yin, R., Wu, H., Wang, Z., Zhai, Y., Kim, K., Do, C., Matyjaszewski, K., and Bockstaller, M. R. (2023). "Sequence-enhanced self-healing in "Lock-and-Key copolymers." *ACS Macro Letters*, 12(4), 475-480. <https://doi.org/10.1021/acsmacrolett.3c00055>

APPENDIX A. COMMUNITY PARTICIPATION

In May 2024, the Basic Energy Sciences Advisory Committee evaluated future construction projects proposed by the U.S. Department of Energy’s Office of Basic Energy Sciences, including the Second Target Station (STS). The committee recognized STS as having “the potential to be absolutely central to future world-leading science,” but recommended that “the science case must be more fully developed to specify the currently inaccessible grand challenges that the new capabilities can address.”

To address this recommendation, a committee comprising Professors Alan Tennant, Laura Greene, Norman Wagner, and Soichi Wakatsuki was formed in June 2024. A national workshop, titled “STS Grand Challenges Workshop,” was held August 24–26, 2024, in Arlington, Virginia, to gather leading experts and early-career scientists from nearly every scientific field impacted by neutron scattering. The participants evaluated the importance and future benefits of the unique capabilities of neutrons and STS, focusing on scientific challenges that cannot be addressed without this facility. The participants developed writing teams whose input formed the foundation of the grand challenge chapters of this report. Subsequent meetings and surveys—such as the *Second Target Station and Instrumentation Workshop* at the American Conference of Neutron Scattering on June 28, 2024, and the *SNS-HFIR User Group (SHUG) Town Hall: Community Feedback on the STS Grand Challenges* on November 26, 2024—along with contributions from Oak Ridge National Laboratory (ORNL) staff, form the basis for the final report.

National Workshop: STS Grand Challenges Workshop, August 24–26, 2024, Sheraton Pentagon City Hotel, Arlington, Virginia

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Angela Pitenis	UC Santa Barbara	Angus Wilkinson	Georgia Institute of Technology
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Christina Hoffman	Oak Ridge National Laboratory	Christopher Watson	Defense Advanced Research Projects Agency
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This report is the product of a collective effort, and we extend our heartfelt thanks to all who contributed. Each individual's insights and hard work have been crucial in shaping this document, reflecting the true spirit of collaboration. We appreciate every contributor's dedication in making this endeavor a success.			
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STS Grand Challenges Workshop

August 24-26, 2024
Sheraton Pentagon City Hotel

Time	Event/Activity	Location
August 23, 2024		
6:00pm – 9:00pm	Evening Reception and Registration	Cavalier Ballroom
August 24, 2024		
7:30am – 8:30am	Breakfast	Cavalier Ballroom
8:30am – 8:45am	Welcome and Workshop Charge <ul style="list-style-type: none"> - Laura Greene (Florida State University National High Magnetic Field Laboratory) - Alan Tennant (University of Tennessee, Knoxville) - Norm Wagner (University of Delaware) - Soichi Wakatsuki (Stanford University) - Jens Dilling (Oak Ridge National Laboratory) 	Commonwealth Ballroom (South)
8:45am – 9:15am	Vision for a Second Target Station <ul style="list-style-type: none"> - Alan Tennant (University of Tennessee, Knoxville) 	Commonwealth Ballroom (South)
9:15am – 9:45am	Quantum Materials <ul style="list-style-type: none"> - Satoru Nakatsuji (University of Tokyo) 	Commonwealth Ballroom (South)
9:45am – 10:15am	Soft Matter & Polymers <ul style="list-style-type: none"> - Norm Wagner (University of Delaware) 	Commonwealth Ballroom (South)
10:15am – 10:30am	Break	
10:30am – 11:00am	Materials & Engineering <ul style="list-style-type: none"> - Suresh Babu (University of Tennessee, Knoxville) 	Commonwealth Ballroom (South)
11:00am – 11:30am	Chemistry & Environmental Science <ul style="list-style-type: none"> - Roberto Car (Princeton University) 	Commonwealth Ballroom (South)
11:30am – 12:00pm	Biological Materials, Systems & Human Health <ul style="list-style-type: none"> - Kalina Hristova (Johns Hopkins University) 	Commonwealth Ballroom (South)

Time	Event/Activity	Location
12:00pm – 12:30pm	Working Lunch	Commonwealth Ballroom (South)
Breakout Sessions		
12:30pm – 2:30pm	Short presentations and discussions (group)	
2:30pm – 2:45pm	Break	
2:45pm – 4:45pm	Discussions of grand science challenges and identify priority science opportunities (group)	
4:45pm – 5:15pm	Break	
5:15pm – 6:00pm	Short reports from breakout session chairs (all)	
6:00pm – 6:30pm	Break	
6:30pm – 8:00pm	Dinner provided (all)	Commonwealth Ballroom (South)
6:30pm – 8:00pm	Breakout session chairs coordination meeting (make dinner plate and walk over to breakout room)	North 1
Sunday, August 25, 2024		
7:30am – 8:30am	Breakfast	Commonwealth Ballroom (South)
Plenary Presentation		
8:30am – 9:00am	Past Lessons and Future Possibilities - Roger Pynn (Indiana University, Bloomington)	Commonwealth Ballroom (South)
Breakout Sessions		
9:00am – 10:20am	New breakout discussions: Water, AI, Interfaces & Surfaces, Sustainability, Facilities of the Future, Extreme Conditions (groups)	
10:20am – 12:00pm	Discussions on meeting scientific needs and identify priority science capabilities (groups)	

Time	Event/Activity	Location
Plenary Presentation		
12:00pm – 12:30pm	Artificial Intelligence transforming Science - Jared Kaplan (ANTRHOP\C)	Commonwealth Ballroom (South)
12:30pm – 1:00pm	Working Lunch	Commonwealth Ballroom (South)
Breakout Sessions		
1:00pm – 4:15pm	Writing Session 1: Grand science challenges and required experimental and scientific tools (groups) + ad hoc working group on crosscuts	
4:15pm – 5:15pm	Short reports and open discussion (all)	
5:15pm – 6:00pm	Summary: Vision and next steps (all)	
6:00pm – 7:00pm	Working dinner provided (all) – CASH BAR	
Monday, August 26, 2024		
7:30am – 8:30am	Breakfast	Commonwealth Ballroom (South)
Breakout Sessions		
8:30am – 12:00pm	Writing Session 2: Grand science challenges and required experimental and scientific tools (groups)	

Breakout Session, Chairs, and Co-chairs

Quantum Materials: Collin Broholm (chair, Johns Hopkins University), Mingda Li (co-chair, MIT)

Soft Matter & Polymers: Nitash Balsara (chair, UC Berkeley), Nairiti Sinha (co-chair, Pennsylvania State University)





































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Biological Materials, Systems & Human Health: Eddie Snell (chair, Hauptman-Woodward Medical Research Institute), Jonathan Nickels (co-chair, University of Cincinnati)

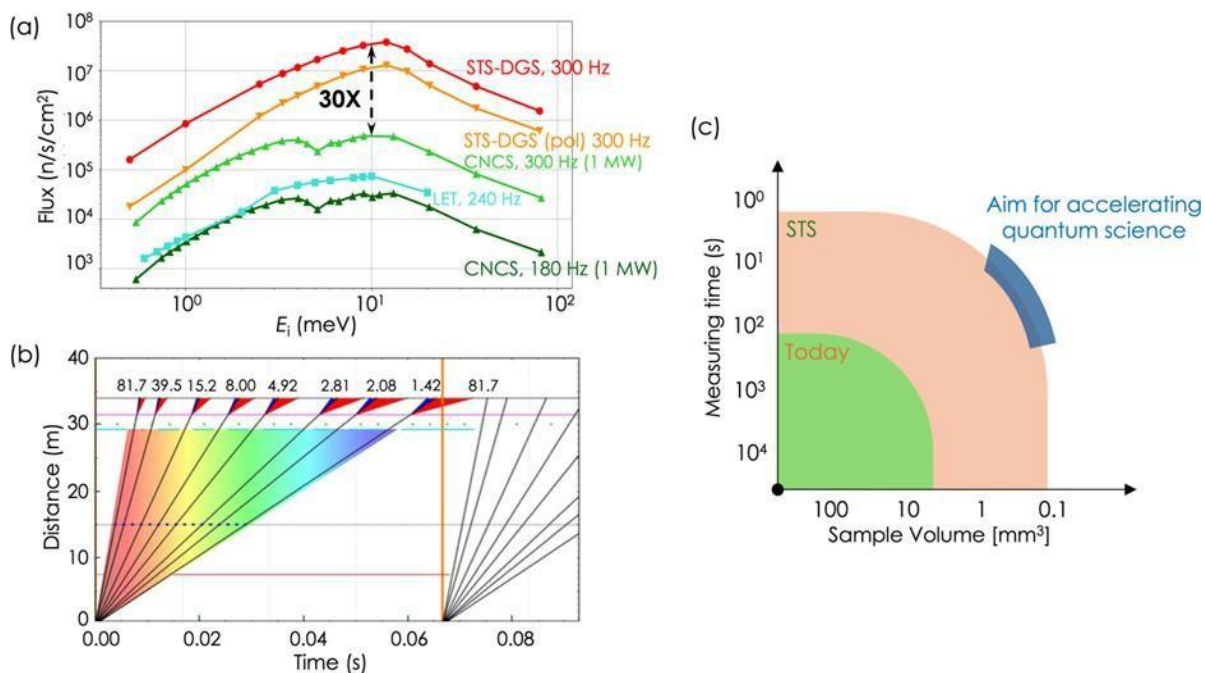
APPENDIX B. REFERENCE SECOND TARGET STATION INSTRUMENT SUITE

The following figure describes the unique capabilities of neutron instruments at the Second Target Station (STS) and describes the science themes covered by each of the key technique areas.

Neutron Scattering	Unique STS instrument capabilities	Science Theme Areas	
Spectroscopy Indirect geometry	$S(q, \omega)$ from 10nm thin films & heterostructures	    	 Magnetism
Spectroscopy Direct geometry	Microgram samples Rep Rate Multiplication & Per Pulse measurements	   	 Quantum entanglement
Powder & Single Crystal Diffraction	Microgram Samples Extended d spacing range. Per pulse measurements	   	 Crystallography
Engineering Diffraction	Extended d spacing range. Per pulse measurements	 	 Chemistry
Neutron Imaging	Micron resolution NGI. Real Time multiscale volume reconstruction	   	 Material Engineering
SANS	Per pulse measurement. Extended Q range Focus Beams	    	 Civil Engineering
Reflectometry	Per Pulse NR measurements	   	 Life science
			 Structural Biology

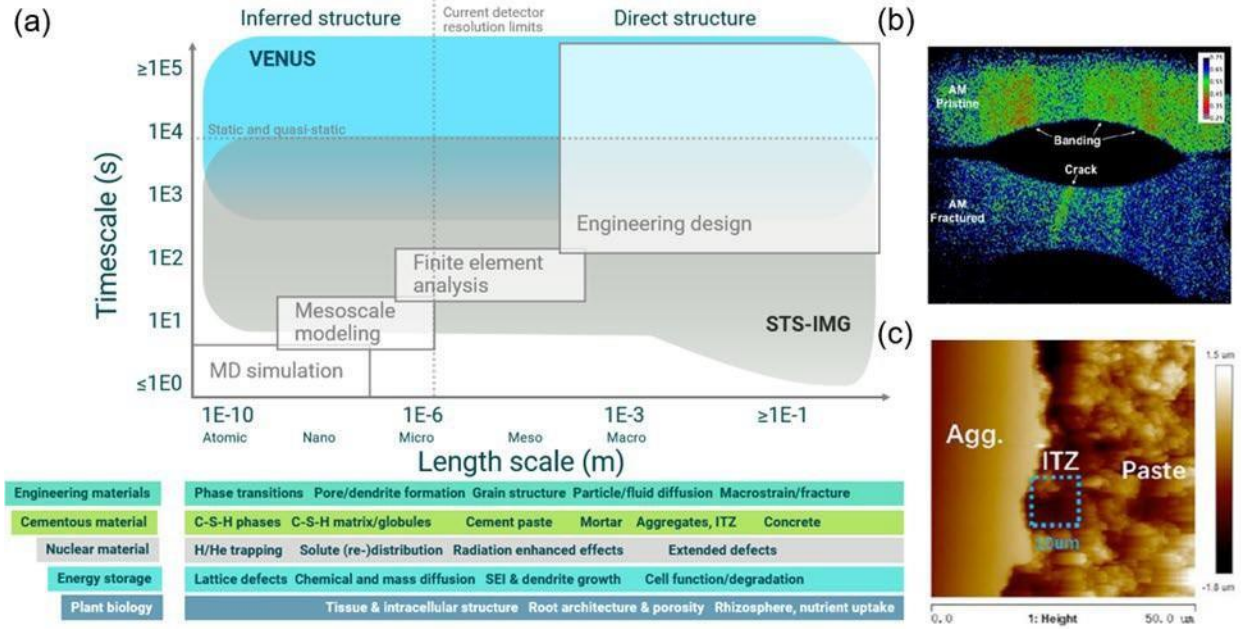
Following are detailed descriptions of the performance characteristics for a reference STS instrument suite for diffraction, imaging, inelastic scattering, and large-scale structures research.

Inelastic Neutron Scattering for Functional and Quantum Materials at STS



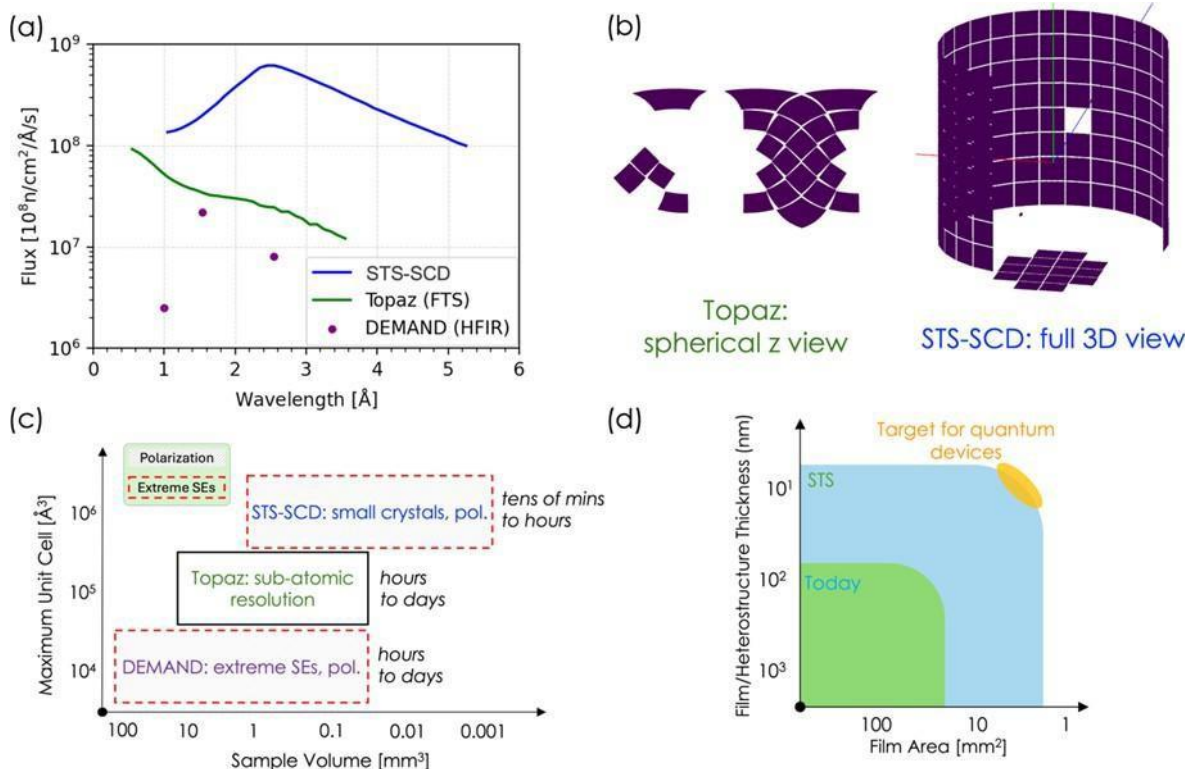
An STS direct geometry neutron chopper spectrometer (STS-DGS) will enable spectroscopic measurements on materials with crystals smaller than 1 mg. (a) Leveraging STS's high source brightness and advanced focusing optics, STS-DGS delivers 30-fold higher flux in monochromatic mode over CNCS, a world-class cold neutron spectrometer at the Spallation Neutron Source First Target Station. (b) Its innovative repetition rate multiplication technique, unavailable at CNCS, harnesses STS's low source frequency to provide up to eight incident energies from a single pulse, significantly boosting data acquisition. (c) STS-DGS will provide transformative capability to accelerate quantum science by enabling the study of much smaller samples. A detector array, covering 2π steradians (3.6 times the solid angle of CNCS), is housed in a large vacuum vessel to minimize background and maximize sensitivity to weak signals. Overall, STS-DGS will achieve a data collection rate about 500 times higher than CNCS at equivalent resolutions (accounting for a conservative 0.6 efficiency factor: $30 \times 8 \times 3.6 \times 0.6$). The design also will enable experiments under extreme conditions, such as low temperatures, high magnetic and electric fields, and high pressures. Furthermore, STS-DGS's high flux will fully exploit XYZ polarization analysis, a powerful tool that measures all components of the full polarization tensor $S_{\alpha\beta}(Q, \omega)$. This technique will enable groundbreaking advancements in quantum magnetism research by providing crucial insights into complex magnetic phenomena in bulk and at interfaces and devices. These insights will drive the development of novel functionalities that underpin emerging information and technologies, moving from materials to devices and prototypes. STS-DGS will integrate AI-driven methods to optimize measurements, including determining counting times and experimental strategies. AI methods will efficiently map the four-dimensional $S(Q, \omega)$ function, maximizing information content without necessitating exhaustive full mapping. Additionally, AI will optimize the numerous configurations needed for polarized spectroscopy and analyze comprehensive datasets generated by repetition rate multiplication. These AI-driven features will significantly increase throughput and expand the impact of neutron spectroscopy.

New Capabilities of the STS Neutron Imaging Capabilities



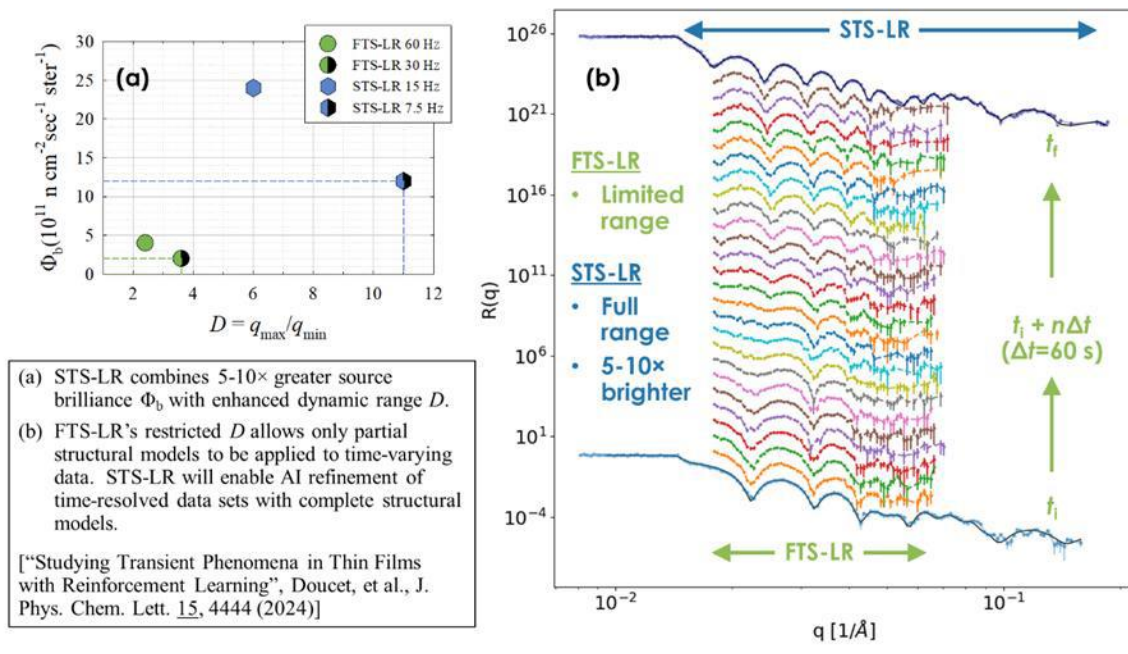
A neutron imaging instrument at STS (STS-IMG) will be a multimodal beamline optimized to capture kinetics of natural and engineered materials that span broad length (angstroms to centimeters) and time scales (seconds to minutes). This new concept features a 40-fold increase in flux of cold neutrons over a wider wavelength band (7.9 Å vs. 5.3 Å) than currently accessible at VENUS at the First Target Station. (a) Unique capabilities: High source brightness combined with simultaneous Bragg edge imaging (BEI) and neutron grating interferometry (nGI) unlocks imaging of the mesoscale, which is rich with heterogeneous structures in real materials that current multiscale physics models struggle to capture, such as the distribution of fine particles and their displacements under load. STS-IMG will excel at coupling microscopic and macroscopic length scales, allowing for more accurate and efficient up- or down-sampling of relevant material properties. (b) In situ and operando systems: By design, STS-IMG will enable study and, in many cases, quantification of transient, irreversible, and time-evolving microstructures like structural phase transitions, hydrogen diffusion and embrittlement, pore formation, fatigue, and corrosion, with the ability to correlate with external stimuli like mechanical load, magnetic field, atmosphere, temperature, and pressure. Studies of crack initiation in additively manufactured parts, for instance, consist of time-evolving microstructures under mechanical load wherein dark-field contrast provides early indication of crack formation and diffraction contrast via BEI reveals changes in material phase near crack boundaries. (c) Multiscale structures: Buried interfaces influence material properties on the macroscale, such as the interfacial transition zone in cement. Through simultaneous BEI and nGI, compositional, crystallographic, and microstructural information of these structural scales are combined and spatially resolved (i.e., pixelated) in each 2D snapshot. Therefore, these characteristics can be carried into 3D via tomography, unlocking true tensorial tomography (strain and magnetic) as well as digital twins of materials on the component scale.

New Capabilities of the STS Single-Crystal System

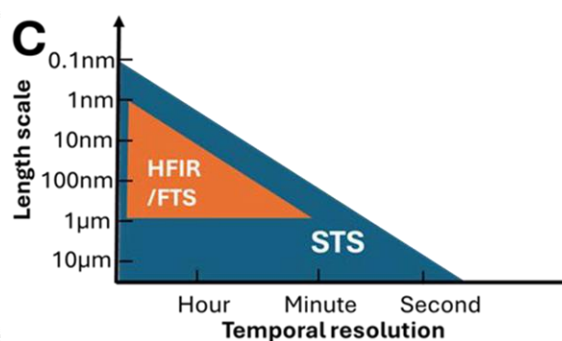
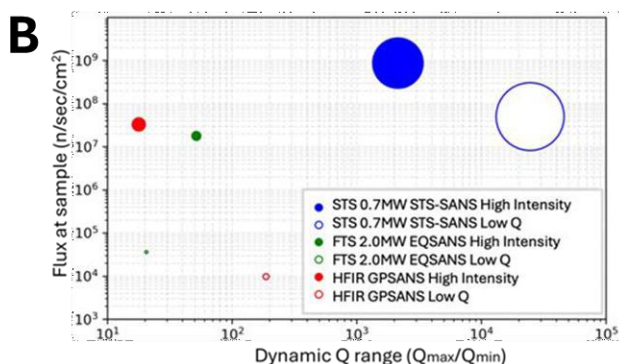
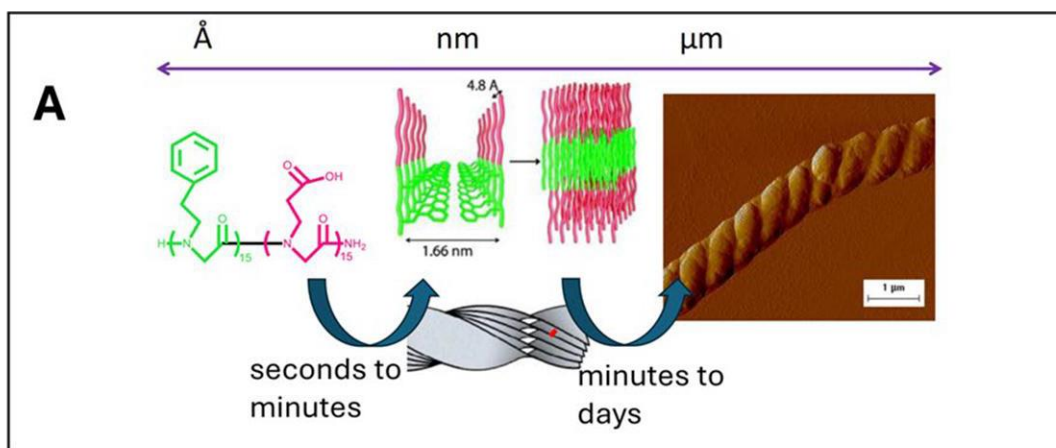


An STS single-crystal diffractometer (STS-SCD) will enable single-crystal neutron diffraction with a performance gain factor of 180 compared with TOPAZ at the First Target Station (FTS) coupled with broadband polarization diffraction capabilities. (a) Flux: STS-SCD will deliver approximately 30 times higher absolute flux than TOPAZ at FTS, leveraging a broader wavelength band (4.3\AA vs. 3.1\AA) and enhanced wavelength-resolved flux. Compared with DEMAND at the High Flux Isotope Reactor (HFIR), this gain is even more significant. Targeting materials with larger characteristic length scales, STS-SCD's use of longer wavelengths will further enhance effective flux by a factor of 3, given that reflection probability scales with the square of the wavelength, and detector efficiency improves with colder neutrons. (b) Detector: Whereas TOPAZ employs a quasi-spherical detector geometry with 25 banks at about 0.43 m from the sample, covering 3.2 steradians with 1.64 million pixels, STS-SCD's quasi-cylindrical detector geometry will feature 175 banks at about 0.80 m from the sample. This setup covers 6.6 steradians with up to 25.8 million pixels, yielding a $2\times$ increase in solid angle coverage and an $8\times$ improvement in solid angle resolution. (c) Capabilities: STS-SCD's higher flux and expanded solid angle coverage will enable measurements on samples $1/50$ the size allowed by current instruments at the Spallation Neutron Source and HFIR. It can analyze complex materials with $10\times$ larger unit cells owing to improved resolution. The increased sample-to-detector distance will accommodate versatile sample environments and allow for the use of scattering beam collimators to improve signal-to-noise ratio. Additionally, STS-SCD will provide a polarized beam option, filling a critical gap in broadband polarization diffraction capabilities in United States peer instruments such as SENJU at the Japan Proton Accelerator Research Complex, WISH at ISIS, and MAGIC (under construction) at the European Spallation Source, all of which include polarization capabilities. (d) Quantum device research: STS-SCD will provide high-fidelity data on ultrathin films and interfacial materials in heterostructures such as twistrionics, a key to advancing quantum technologies. These samples, often only nanometers thick and square millimeters in area, remain beyond the reach of existing neutron scattering instruments at FTS and HFIR.

New Capabilities of the Large-Scale Structure at STS Reflectometry and Small-Angle Neutron Scattering



A liquids reflectometer at STS (STS-LR) will enable reflectivity measurements by making time-dependent measurements. In terms of speed, STS-LR will collect data 25× faster than the FTS LIQREF instrument. However, more important than that raw gain is the way in which STS-LR will operate, enabled by the unique characteristics of STS. (a) Brilliance and dynamic range: STS-LR, viewing the compact STS cylinder moderator, will deliver 5–10 times higher brilliance on sample than LIQREF. This intensity will be delivered at 15 Hz and will be distributed over a three times larger wavelength bandwidth than is available at LIQREF. (b) Capabilities: STS-LR's combination of high brilliance delivered over a broad-wavelength bandwidth results in qualitatively different performance because it enables collection of complete datasets in a single instrument setting (i.e. “cinematic” operation). Unlike LIQREF, which can fit only partial structural models to its truncated datasets, STS-LR will function as a camera, collecting data from a changing sample at frame rates as rapid as a single accelerator pulse. Research opportunities: STS-LR will serve a broad scientific community. The ability to collect single-setting complete datasets quickly presents both a challenge and an opportunity. The difficulty of analyzing large time-evolving datasets are driving the development of ML-based analysis (see reference in figure above). STS-LR will generate such data >25× faster across Q -ranges, allowing full profile refinement. This capability will revolutionize neutron reflectometry: every measurement will potentially be a time-dependent or parametric measurement, and data analysis will no longer fall solely on the individual researcher. Exciting applications are foreseen in such areas as in situ time-resolved measurements of electrochemical production of ammonia, redox reactions at surfaces, corrosion in advanced reactor vessels, polymer diffusion and reaction processes, and protein interactions with cell membranes.



A small-angle neutron scattering instrument at STS (STS-SANS) exemplifies the revolutionary leap in cold neutron peak brightness across a wide usable wavelength band at STS. STS-SANS will enable simultaneous, subsecond time-resolved probing of atomic- to mesoscale structure evolution (e.g., Q -range of $0.001\text{--}20 \text{ \AA}^{-1}$) in hierarchical systems under in situ or operando conditions. (A) Kinetic insights into hierarchical assemblies: Hierarchical materials, such as polymers, self-assemble dynamically across six orders of magnitude in time (seconds to days) and length scales (angstroms to micrometers). For instance, bioinspired peptoid diblock copolymers form monodisperse superhelices through a hierarchical process highly sensitive to molecular charge. (Illustration adapted from <https://pubs.acs.org/doi/10.1021/ja106340f>). Spin-echo modulated SANS will extend the range of instrument sensitivity to tens of micrometers. STS-SANS will measure angstroms to tens of micrometers and seconds to days in a single measurement (represented by the blue region in [C]), offering unprecedented insights into assembly mechanisms by capturing intermediate structures of all relevant length scales between primary assemblies and final superstructures. (B) Performance gain in flux and dynamic Q -range (defined as $Q_{\text{max}}/Q_{\text{min}}$): Compared with FTS EQ-SANS in the high-intensity mode, for example, STS-SANS will offer $50\times$ higher flux and $40\times$ broader dynamic Q -range. At the low- Q mode, STS-SANS will provide an astounding $1,400\times$ flux and $1,200\times$ dynamic Q -range (the size represents the maximum Q reachable). (C) Temporal and spatial ranges: STS-SANS will push beyond the boundary of current capabilities to enable groundbreaking observation of molecular assemblies, revealing critical early-stage intermediates that drive the formation of final structures.