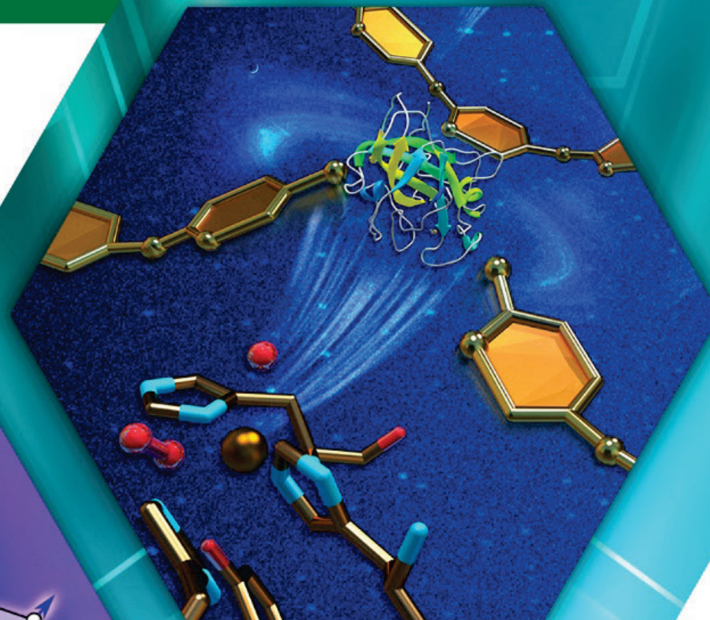
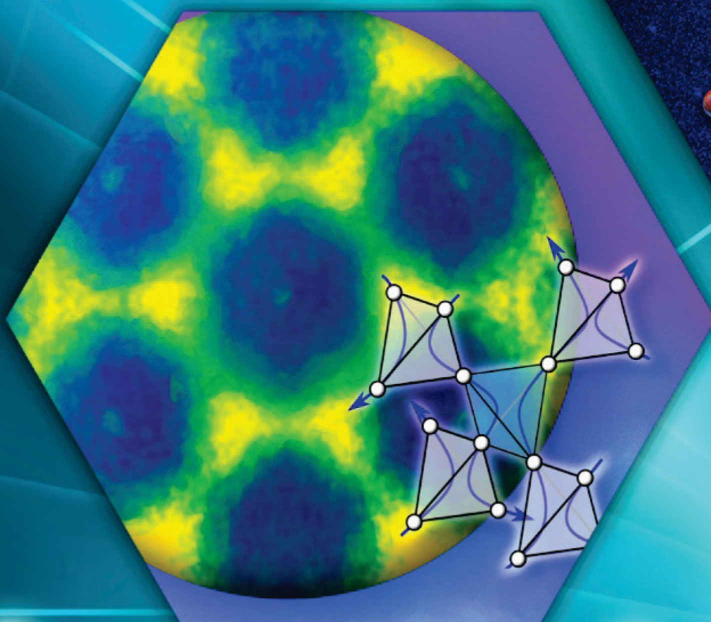
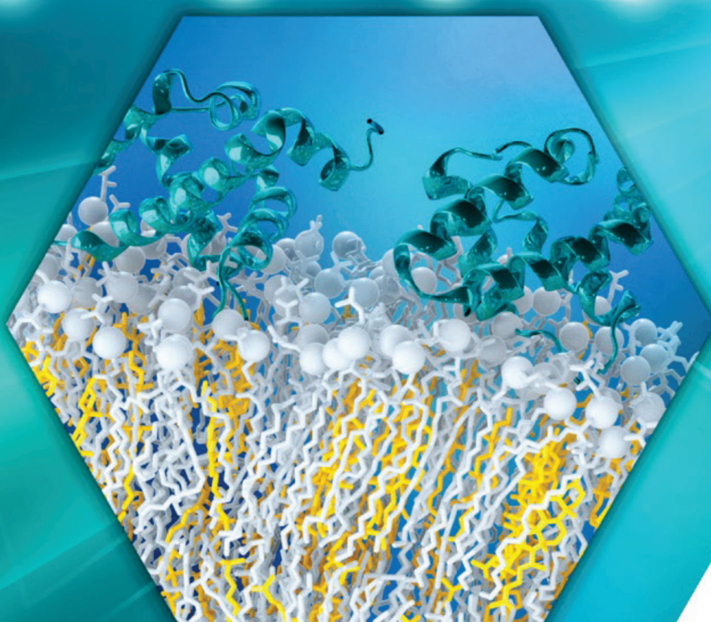
FIRST EXPERIMENTS

New Science Opportunities at the Spallation Neutron Source Second Target Station







Oak Ridge National Laboratory

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FIRST EXPERIMENTS:

New Science Opportunities at the Spallation Neutron Source Second Target Station

This brochure is an abridged version of a more comprehensive companion report.

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Scattering Neutrons, Harvesting Knowledge

High-Brightness Cold Neutrons for Materials Discovery and Innovation

The ability to probe the structure and dynamics of materials, beginning at the atomic level and extending to objects well beyond the nanometer scale, is essential to the development of future technologies that will drive this nation's economy—new batteries and structural materials for transportation, new catalysts for efficient production of fuels and chemicals, next-generation polymers that make it possible to upcycle waste into new consumer products, and quantum materials to enable advances in computing and sensors.

The mission of the Office of Science of the US Department of Energy (DOE) is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States. To carry out this mission, the Office of Science develops and operates a remarkable set of scientific user facilities. These tools for scientific discovery and innovation, used by thousands of scientists annually, include some of the world's best resources for understanding and characterizing materials at the level of atoms and molecules. The Office of Science has developed powerful sources of x-rays and neutrons, including five x-ray light sources and two neutron scattering facilities, and provides additional capabilities at five nanoscale science research centers that include advanced electron microscopies. Experiments conducted using these scientific tools have extended the frontiers of science and led to new technologies with real-world applications.

Neutrons are a unique tool to study materials: because they carry no electrical charge, they interact directly with the nuclei in a material and are sensitive to light elements as well as isotopic differences; neutrons carry a magnetic moment and thus directly interact with magnetic structure and excitations; and because they penetrate deep into materials, they can be used to study samples inside pressure or reaction vessels. Neutrons also have energies similar to those of many lattice vibrations, molecular motions, and magnetic excitations. (See the sidebar "Why Neutrons" on p. 4) The two neutron sources in the United States supported by the DOE Office of Science, the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS), are both located at Oak Ridge National Laboratory (ORNL).

- Operating at 85 MW, HFIR provides a steady-state neutron flux as high as that of any research reactor in the world. HFIR produces continuous beams of either cold or thermal neutrons. It has 12 instruments available to the user community.
- At SNS, a 1.4 MW accelerator drives the production of 60 pulses of neutrons per second (60 Hz) at the First Target Station (FTS). These high–peak brightness neutrons, which are tailored for high energy resolution, are delivered to a suite of 19 instruments. An upgrade under way at SNS will double the power capability of its accelerator to 2.8 MW by 2024.

STS: Securing US Leadership in Neutron Scattering

DOE proposes to build a Second Target Station (STS) at SNS to produce beams of cold neutrons with world-leading peak brightness at a repetition rate of 15 Hz, providing broad energy/wavelength ranges that can be used simultaneously. Construction of the STS will provide transformative capabilities that allow thousands of users from national laboratories, universities, and industry to address grand scientific challenges [Hemminger 2015], advance energy research [BES Workshop Reports 2019], and accelerate industrial innovations through the combination of

- Cold (long-wavelength) neutrons of unprecedented peak brightness
- Short neutron pulses with broad ranges of usable wavelengths or energy

This unique combination of neutron beam characteristics will open new avenues for examining materials and systems over greatly increased length, energy, and time scales. These characteristics—in combination with new instruments and sample environments, advances in neutron optics and detectors, and new computational methods—will make it possible to conduct a wide range of experiments not now possible anywhere in the world. Specifically, the STS will provide unique capabilities for experiments that require

- Time-resolved measurements of chemical and physical processes, such as materials as they are being synthesized, processed, or self-assembled; chemical processes at interfaces; and changes in biological macromolecular complexes

- More intense neutron beams focused to explore smaller samples of newly discovered or synthesized materials, or materials under the extreme conditions of magnetic field, pressure, and temperature that are often encountered in energy technologies

- Simultaneous measurements of hierarchical architectures across an unprecedented range of length scales, from atomic scale to the micron and beyond, that will reveal how materials, such as polymers, self-assemble into hierarchical structures and how proteins interact in living biological cells.

The STS will provide transformative new capabilities for many fields of research—materials science, physics, chemistry, geology, biology, and engineering, among others. The section "Science Enabled by STS" presents examples of opportunities to apply these capabilities to challenges in five key areas of science: polymers and soft materials, quantum matter, materials synthesis and energy materials, structural materials, and biology and life sciences.

The STS Project, now in progress at ORNL, will design, construct, install, and commission the facilities and equipment needed to create a world-leading source of cold neutrons of unprecedented peak brightness at SNS. Key aspects of the STS design, including preliminary descriptions of an illustrative suite of eight instruments, are presented in the section "The STS at SNS."

The capabilities offered by the STS instruments (22 when fully built out) will complement those of the FTS and HFIR, providing the United States with unparalleled resources for neutron scattering at the world's leading high–peak brightness cold neutron source as shown in Fig. 1.

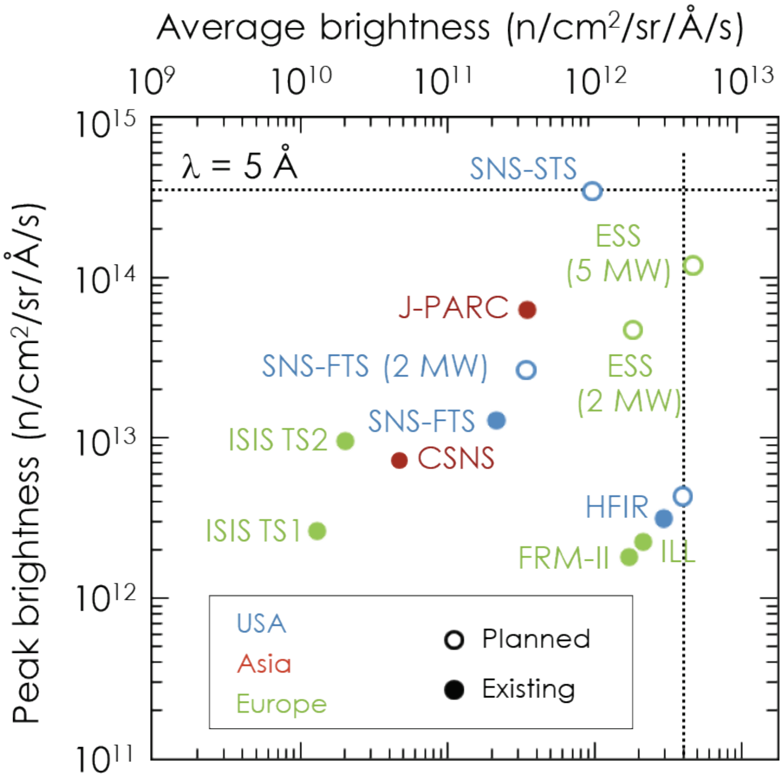

Fig. 1. Peak and time-averaged brightness of existing (closed circles) and planned (open circles) sources of cold neutrons (wavelength λ = 5 Å). CSNS: China Spallation Neutron Source, China; ESS: European Spallation Source, Sweden; FRM-II: Forschungsreaktor München II, Germany; ILL: Institut Laue-Langevin, France; ISIS: ISIS Neutron and Muon Source, UK (TS: Target Station); J-PARC: Japan Proton Accelerator Research Complex, Japan. *Image source: ORNL*.

The International Landscape for Accelerator-Based Neutron Sources

Powerful new accelerator-driven neutron sources in other nations include the neutron source at the Japan Proton Accelerator Research Complex (J-PARC), a short-pulse source operating at 25 Hz with a design power of 1 MW, and the European Spallation Source (ESS), a long-pulse source to be operated at 14 Hz and 2 MW when construction is completed in 2025 (with plans for an upgrade to 5 MW in the future). The lower repetition rates of J-PARC and ESS will allow the use of broader ranges of neutron energies in each pulse compared with FTS. The long pulses of neutrons at 14 Hz at ESS will provide both high peak brightness and a broad range of neutron energies (a strength of short-pulse spallation neutron sources with low repetition rates) and high time-averaged fluxes of both cold and thermal neutrons (a strength of reactor-based sources).

Why Neutrons?

Neutrons' specific properties provide unique insights into the structure and function of materials. Because neutrons have no electrical charge, they have higher penetrating power than electrons or x-rays; this property enables the study of bulk materials (such as structural materials) and buried interfaces, chemical processes (such as catalysts) in high-pressure reaction vessels, and even the operation of fuel injectors in an operating engine. Neutrons also have a magnetic moment, making them an especially sensitive probe of magnetic properties in quantum materials and other magnetic materials. Whereas beams of x-rays and electrons interact with the electrons in an atom, neutrons interact directly with atomic nuclei, making them uniquely sensitive to the detection of many light elements, such as hydrogen. Further, they can distinguish among different isotopic forms of some elements. This unique feature can be exploited to follow biological processes to understand, for example, how nature produces fuels using sunlight in photosynthetic processes; it also enables observation of the self-assembly of polymers into functional architectures that can be exploited for water purification and other applications. Neutrons can be produced with a wide range of wavelengths suitable to probing structures from the atomic level through 100s of nanometers and beyond, and they have energies well matched to studying both collective and individual atom motions. Finally, neutrons interact with both nuclei and magnetic fields in quantitative ways that support direct comparison between experiment and theoretical and computational modeling.

The use of neutrons to probe the structure and dynamics of materials began in the 1940s with the construction of the first nuclear reactors. Neutrons extracted from these reactors were directed to scientific instruments, where their interactions with target materials were studied. The construction of more powerful reactors and the development of accelerator-based neutron sources, combined with advances in neutron instrumentation and techniques, increased the utility of neutrons as a research tool, leading to notable advances in both basic and applied research and development. Neutron scattering studies like the following have been vital to a detailed understanding of many materials and their properties:

- advancing new high-temperature superconductors and quantum materials
- examining enzymes in drug-resistant bacteria that play a role in modifying antibiotics, rendering them ineffective
- developing magnetic materials used in data storage, personal electronics, and power generation and transmission
- increasing the performance of polymers by adding nanoparticles
- improving the reversible charge-discharge capacity in novel batteries

Today's most powerful neutron sources include both research reactors, which typically produce continuous beams of neutrons with high time-averaged brightness, and accelerator-based spallation sources, which typically produce pulsed beams of neutrons with high peak brightness. Both can be optimized to provide neutron beams with characteristics best suited to the material structures and interactions being studied.

Generally speaking, it is desirable to match neutron energies and wavelengths to the energy and length scales, respectively, of the materials under investigation. The energy of the neutrons produced must be reduced to make them useful for neutron scattering experiments. Thus, they are passed through a moderator that removes most of their kinetic energy by collisional cooling. The energy of the moderated neutrons is then characterized by the temperature of the moderator.

- Thermal (i.e., room-temperature) neutrons have wavelengths of ~1.8 Å (a few tenths of a nanometer) and energies of ~25 meV. These characteristics make them useful for investigating atomic length scales and measuring the vibrational energies of atoms in a crystal lattice.
- Cold neutrons with lower energies (~3 meV) and longer wavelengths (~5 Å) are useful for studying large-scale structures (e.g., watching polymers self-assemble into intricate architectures) and low-energy excitations (e.g., excitations in frustrated systems and various problems in magnetism, superconductivity, and correlated electron systems). Because they reflect well from surfaces, they can also be transported over long distances with minimal losses and be focused to small beam sizes.

The increasing use of neutrons in various areas of science is driving demand for additional resources and improvements in the precision and resolution of measurements that can be made with neutrons. A source of high-brightness cold neutrons that can simultaneously access a broad range of energies and wavelengths will provide the scientific community with exciting new opportunities to examine, understand, and improve a variety of materials.
Adapted from Pynn, R. Neutron Scattering: A Primer. Los Alamos Science 1990, No. 19, 1–31.

Science Enabled by the STS

The scientific community has evaluated opportunities to apply the capabilities of the STS to emerging challenges in a variety of fields. The examples presented in this section span polymers and soft materials, quantum matter, materials synthesis and energy materials, structural materials, and biology and life sciences, illustrating the extraordinary potential of the STS to impact a broad spectrum of scientific fields.

Polymers and Soft Materials

Polymers and soft matter self-organize through very weak interactions into larger structures, creating hierarchically structured materials with macroscopic properties stemming from the interplay of the structures found at different length scales. Because these structures can be altered through changes in temperature, pressure, stress or flow, soft materials are more readily tailored than most other materials, thereby affording new ways to create a desired structure or function.

Neutron scattering is a key tool for studying polymers and soft materials because neutrons can penetrate reaction vessels, allowing in situ measurements to monitor reaction processes, without destroying the relatively weak bonds in the materials. In addition, neutrons have strong sensitivity to both hydrogen and deuterium but can readily differentiate between the two to provide insight into reaction mechanisms and structure. These capabilities, combined with the high flux and broad energy range provided by the STS, will provide transformative capabilities to probe transient, time-dependent, and nonequilibrium processes in soft materials, with measurements completed in seconds or less, including

- high peak brightness and pulse structure that allow monitoring of the evolution of out-of-equilibrium states
- simultaneous characterization at length scales from the atomic level up to the emerging nanoscale and mesoscale hierarchical architectures
- simultaneous resolution of length and time scales, particularly when combined with specific contrast to identify soft molecular interactions and cooperativity

A fundamental question in polymer science and technology is

> *How can we control the assembly of soft matter to realize a wholly new generation of dynamic, hierarchical, polymorphic, and reconfigurable materials?*

Answering this question would allow scientists to design soft materials with functionality approaching that of natural systems or even to design polymers with superior properties that can be readily recycled to create new high-value materials.

For example, coacervate complexes are formed from charged polymers that self-assemble (Fig. 2) as a result of mainly electrostatic attraction between oppositely charged polymers. These materials are of high interest because they can respond to “triggers” in ways that cause their functionality to change. For instance, they could be employed to deliver specific “cargoes,” such as ions in batteries (triggered with electric fields) or drugs for medical applications (triggered with changes in pH). These materials could form the foundation for production of robust smart materials that strengthen upon application of strain or self-heal by forming new chemical bonds.

Today, the processes by which polymer chains respond during coacervation remain largely unknown. But understanding the formation pathways is critical to being able to design these materials to provide desired functionality. Neutrons are well suited to probing such systems, but observing the relevant length scales with a time resolution of seconds or below is not currently possible. The capabilities of the STS, including a new generation of instrumentation, will enable the study of these processes over wide time and length scales with a real-time resolution of seconds. With these world-leading capabilities, researchers can finally decode this longstanding mystery and unlock our ability to predictively design these 3D structures to deliver highly functional coacervate materials.

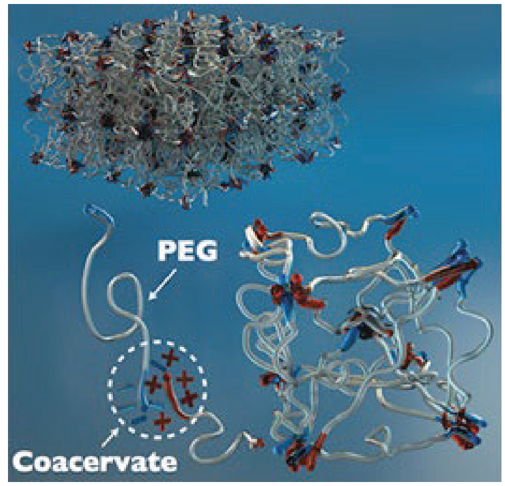

Fig. 2. Schematic of an ABA block copolymer complex coacervate. The oppositely charged A blocks create the coacervate (lower left). The coacervate domains are bridged by the neutral B block (here polyethylene glycol, or PEG). The coacervate domains can adopt a loose gel-like structure (lower right) that can become very well ordered at the nanoscale (top left) if concentrations are high enough [Srivastava et al. 2017]. The time evolution of such systems will be observable with the capabilities available at the STS. *Image source: Courtesy of Peter Allen, Institute for Molecular Engineering, University of Chicago.*

New scientific opportunities

The new capabilities provided by the STS will revolutionize our ability to understand nanoscale changes in soft materials with neutrons. They will provide new opportunities for the study of time-resolved phenomena associated with the processing, 3D printing, or assembly of complex polymers, soft materials, and nanomaterials. As a result, these next-generation instruments will lead to breakthroughs in the development of responsive, recyclable, and reconfigurable materials for future energy technologies such as photovoltaics, fuel cells, batteries, lightweight materials, lubrication, gas purification, water desalination, and microelectronics and computing.

Quantum Matter

Quantum materials hold exceptional promise for the development of next-generation computers, high-precision sensors, and new energy technologies. Examples of quantum materials include superconductors, in which electrons form a collective quantum state that carries electricity with no resistive heat losses; topological materials, in which the geometric connectivity of quantum states leads to a novel form of electron transport at surfaces; and superfluids, which can flow with zero viscosity.

Neutron scattering provides unique insight into the workings of these materials because of the sensitivity of the neutron to the magnetism, or spin, of electrons, and the ability of neutrons to probe low-energy fluctuations that determine the behavior of quantum states. The high brightness and wide energy bandwidth provided by the STS will enable studies of new quantum materials at the very earliest stages of discovery and will extend the application of neutron scattering to new classes of materials, such as artificially layered materials, interfaces, or assemblies of nanoparticles that are difficult to access with current neutron sources. Thus, the STS will accelerate the transformation of quantum materials into new technologies with the potential to strengthen national security, create unparalleled computing power, and enhance economic competitiveness.

One of the key questions in quantum materials research is

> *How can quantum fluctuations be controlled and exploited to design new materials for energy-relevant technologies?*

One intriguing example is a quantum spin liquid (QSL), a state in which the motions of highly entangled spins behave like new kinds of particles. Greater understanding of the behavior of these particles may make it possible to deploy them in future technologies. An excellent illustration is provided by a theoretical construct known as the Kitaev model, a network of spins on a honeycomb lattice. This QSL model gives rise to particle-like fluctuations, known as Majorana fermions, that could form the basis of a technology for quantum computing. As materials exhibiting the essential features of the Kitaev model are developed, neutrons will be an essential tool for characterizing and understanding their behavior. Majorana fermions (see Fig. 3) produce a signature that can be seen in a neutron scattering measurement made with the unprecedented resolution, intense beams, and broad bandwidth that will be supplied by the STS.

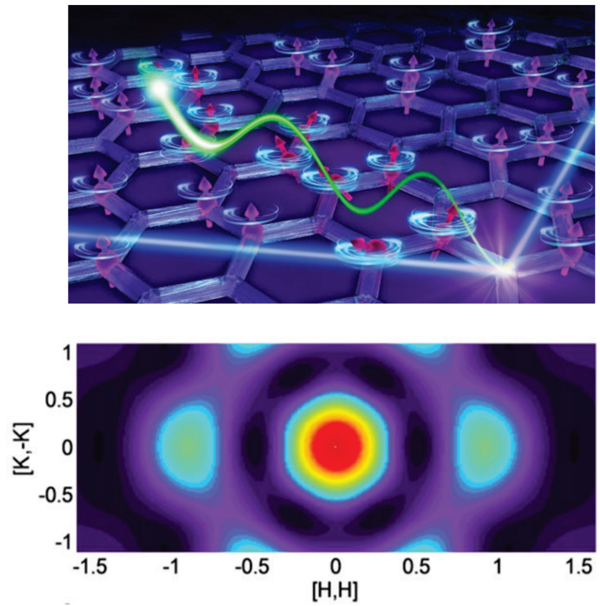

Fig. 3. Using neutrons to explore Kitaev QSLs. Top: Artist's conception of a neutron exciting a Majorana fermion in a Kitaev QSL. *Image source: ORNL.* Bottom: Predicted inelastic neutron scattering pattern for a Kitaev QSL. *Image source: Banerjee et al. 2017.*

New scientific opportunities

The field of quantum materials is growing rapidly and goes far beyond QSLs to include emergent topological states in spin-orbit coupled metals, Weyl semi-metals, axion insulators, and topological Mott insulators. The key characteristics of the STS will enable unprecedented insights into the fundamental physics of these materials, which is critically important for opening pathways to new technologies. For example, the high peak brightness and highly focused beams of the STS will make it possible to perform neutron studies on smaller samples than are currently possible, allowing newly synthesized materials to be examined early in the discovery process. This sensitivity will also make it possible to study layered materials with interfaces designed to enhance quantum properties in devices, providing unprecedented understanding of thermal or magnetic transport across these designed interfaces.

The STS will also make it possible to study quantum materials under extremes of magnetic field or pressure. Under such extreme conditions, new and uniquely detailed information will be obtained on the types of interactions that determine a material's properties. Also, the high peak brightness and energy bandwidth attainable with the STS will facilitate fundamentally new ways of looking at quantum matter. The unrivaled peak brightness of STS will dramatically expand our ability to probe time-dependent processes in materials. For measurements on time scales of seconds or longer, the additional intensity will enable faster measurements with better time resolution. Stroboscopic measurements, when possible, will enable much faster time-resolution on the microsecond to the millisecond scales. Time-resolved measurements at the STS will enable an atomic-level view of quantum materials beyond thermal equilibrium, providing important insights into in operando behaviors that are crucial for the development and application of these materials in computing, sensors, and energy technologies.

Materials Synthesis and Energy Materials

Understanding the chemical processes involved in the synthesis of materials, as well as those associated with energy production, storage, and use, requires the ability to observe and characterize multiple processes simultaneously across broad length and time scales. For example, in the case of energy storage materials used in a battery or supercapacitor, charging and discharging, energy flow, and chemical reactions at the atomic scale are coupled to changes in the electrode structure and to performance of the device at much larger length scales.

Understanding how dissolved species that carry charge interact with the surrounding fluids is also of critical importance. For a battery, this is the interaction of charge-carrying species (e.g., lithium) with the electrolyte (typically an organic liquid). Because both charge carriers and electrolytes are made up of light elements, neutrons provide an exceptionally sensitive means of probing these processes. Further, uncertainties in the chemical reaction mechanisms that occur during the precipitation of solid phases from liquids (e.g., the formation of undesirable secondary phases in a battery that can shorten its lifetime or lead to catastrophic failure), and the subsequent assembly of small particles into macroscopic aggregates, hinder our ability to predict new device performance and develop new materials synthesis strategies.

Neutron scattering is essential to attaining a detailed understanding of materials characteristics and behaviors—including roles of disorder and defects, fluid flow and reactivity, kinetics, materials growth and synthesis, and performance in nonequilibrium and extreme conditions—and to understanding how components and integrated materials in devices function under real-world conditions. Such knowledge is a prerequisite for developing the next generation of energy technologies and understanding hierarchical and heterogeneous structures from the atomic scale to actual components and systems. And transitioning that knowledge to practical uses requires an integrated understanding of synthesis at the nano-, meso-, and macroscale. STS instruments will incorporate multiple modalities by combining different neutron scattering analyses made simultaneously on a single sample, and by combining neutron measurements with those made using other analytical tools. The power and adaptability of the STS beamlines will allow significant advances in the ability to conduct complex experiments in situ and in real time.

Two key questions for designing new energy materials are

> *How are atomic-scale reactions in liquids linked to the macroscopic structure and transport within a material?*
>
> *How we can take advantage of this linkage to design and control energy materials more efficiently?*

The STS will provide wholly new capabilities to address these questions, including the ability to observe processes at different length scales simultaneously and over time. To gain a quantitative and mechanistic understanding of how macroscopic system performance over time is influenced by the atomic-scale structure and reactivity (and vice versa), measurements must be performed in one experiment (see Fig. 4). In addition, increases in cold neutron brightness at STS will allow measurements on materials at far lower concentrations than can currently be studied, opening up these experiments to many more scientifically and technologically relevant material and chemical systems.

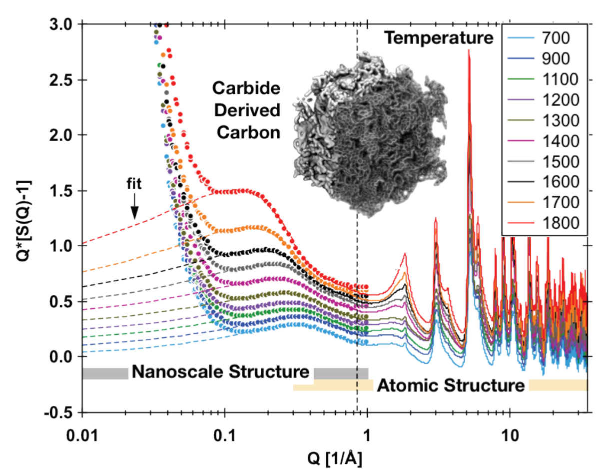

Fig. 4. Simulated neutron scattering data for a potential energy storage electrode material made from carbide-derived carbon. Ex situ measurements of nanoscale and atomic structure have been artificially stitched together to simulate a single data set spanning the size range that will become accessible in a single, time-resolved in situ experiment on STS instruments. *Image source: H.-W. Wang, ORNL; inset: Zhan et al. 2017.*

New scientific opportunities

STS will offer transformative opportunities for capturing the structure and dynamics of complex materials systems in situ and in real time at a temporal resolution of minutes, allowing researchers to follow chemical reactivity self-assembly mechanisms at the atomic/molecular level through transport/aggregation/crystallization toward targeted architectures or functionalities. Doing so will make it possible to establish quantitative links between specific atomic-level solvation structures in solution and reaction pathways during liquid-solid transitions, and then extend these linkages to specific nanoscale morphologies, aggregation behavior, and the ultimate macroscopic crystal form. Without the ability to link relevant reaction and assembly mechanisms across length scales, it will be difficult to control hierarchical assembly and crystallization reactions to tailor specific properties or material morphologies.

Characterizing reactivity, selectivity, and kinetics associated with the reaction and separation of products in solution, under realistic conditions of temperature and pressure, will have a broad impact on DOE missions in science and energy and on the development of new materials and chemical processes for future applications in energy efficiency, production, and storage. The benefits of these new STS capabilities will extend to many processes in which complex aqueous solutions are used, such as treatment of contaminated slurries found in waste tanks, synthesis of materials inspired by biology, and understanding of geological processes [Zhan et al. 2017].

Structural Materials

Structural materials are ubiquitous in modern society as key components in automobiles, airplanes, buildings, bridges, and many more applications. However, today's structural materials realize only about 10% of their theoretical strength. A grand challenge in structural materials is how to increase strength to near-theoretical levels without sacrificing other essential properties, such as ductility and toughness. Solving this challenge would make it possible to realize a new generation of lightweight, high-strength materials. Improvements in the understanding of other aspects of structural materials, including their response to manufacturing and processing (e.g., additive and metamorphic manufacturing processes) and their degradation under extreme conditions (e.g., corrosion and irradiation), could also lead to substantial improvements in performance and to the development of new materials.

Neutrons provide valuable capabilities for studying structural materials, thanks to their deep penetrating power, their ability to monitor atomic-level changes during actual operating and processing conditions, their strong sensitivity to isotopic differences, and, in many cases, their ability to differentiate between elements that are indistinguishable by other characterization techniques. The high brightness and broad energy bandwidths of the STS will advance the study of structural materials by making it possible to

- probe smaller sample volumes to understand complexities and variations in chemistries and macro-structures/microstructure that typically control essential materials properties such as (ion) transport under corrosion conditions, strength, and ultimate functional performance and reliability

- observe transient, time-dependent, and nonequilibrium processes in structural materials, including capturing structural evolution during processing or operation with subsecond time-resolved measurements

- investigate complex and low-symmetry materials and characterize microstructural and crystallographic features across multiple length scales simultaneously

While there are well-established scientific methods for achieving ultrahigh strength in structural materials, in almost all cases they degrade ductility. Only a few notable exceptions have been discovered in which this strength–ductility trade-off is defeated. The exceptions involve either the dynamic generation of certain types of interfaces (twin or phase boundaries) during deformation, or use certain types of nanoscale precipitates or ordered complexes. Broadly speaking, the former approach is better suited for enhancing ductility and the latter for improving strength. A combination of the two is therefore needed to maximize strength and ductility: that is, an optimal distribution of precipitates in a metastable matrix that undergoes twinning and/or phase transformation when stressed or strained (Fig. 5).

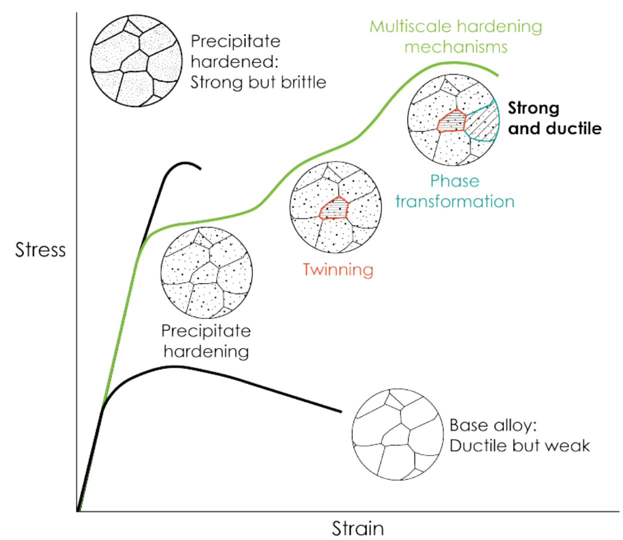

Fig. 5. Strength and ductility. Schematic of interplay between spatial confinement due to precipitates and activation of multiscale hardening mechanisms to achieve high strength and ductility. *Image source: ORNL.*

Although the broad outlines of how to accomplish this combination are known, important scientific questions need to be answered to develop a sound basis for alloy design:

> *Do twin and phase boundaries act merely to provide a steady (or increasing) source of work hardening and thus delay the onset of necking instability, or do they also provide additional deformation modes to accommodate the applied strain and thus enhance ductility?*
>
> *How can the metastability of the matrix, and the volume fractions, morphologies, and sizes of the strengthening precipitates, be controlled to obtain the highest combination of strength and ductility?*
>
> *What are the effects of spatial confinement due to grain boundaries or precipitates on the activation barriers for twinning and stress-induced phase transformations?*

The STS will enable in situ neutron diffraction experiments to study the evolution of relevant microstructural features and load partitioning across length and time scales as a function of strain and temperature. Small-angle neutron scattering (SANS) techniques will provide quantitative measurements of critical precipitate distributions. In combination with theoretical calculations of phase stability and defect energies, these results will help develop broadly applicable scientific principles that can be used to design future generations of stronger and tougher alloys.

New scientific opportunities

The STS will provide exciting new capabilities for structural materials, because it will provide information at high resolution for specific regions in a material while also examining a material across broad length scales. This will allow simultaneous characterization of microstructures, including nucleation and growth of precipitates, metastable phases in complex alloys and composites, long-range order, and defects. The example highlighted in Fig. 5 is a single example of how the STS can help clarify governing mechanisms in next-generation advanced materials, many of which will be increasingly complex and even hierarchically structured. The macroscopic properties of such materials result from multiscale interactions among features from the atomic scale to the microscale. Thus, probes are needed to simultaneously examine those features across those length scales as a function of time. The new capabilities of the STS will enable researchers to conduct entirely new experiments on these advanced materials. Simultaneous measurement of neutron diffraction and SANS data will eliminate the ambiguity of comparing measurements taken with different techniques on different samples. The ability to simultaneously observe these phenomena on time scales similar to those in actual applications is essential to advance our understanding of how a structural material responds to realistic conditions. These insights into structure-property relationships are critical for the design of a new generation of structural materials, improving both the reliability and performance of these materials in transportation, buildings, and many other applications.

Biology and Life Sciences

Natural systems demonstrate a mastery of chemical and physical principles that enables highly selective catalytic processes, efficient energy conversion, and optimized materials synthesis.

The unprecedented peak brightness and broader energy range of neutrons at the STS, with associated advances in neutron optics and detectors, will transform neutron scattering capabilities for biological research. The brightness and energy range of the STS will make it possible to observe changes in biological systems in real time, using smaller samples, and across the multiple length scales relevant to biological systems, from quantum biological phenomena up to cellular scales. Combining the capabilities of the STS with precision deuterium labeling, multimodal experimental environments (or techniques), and high performance computing will allow cinematic observations of collective motions in biomolecular systems and of cellular components as they interact in real time to form functional complexes and higher-order assemblies. A dynamic understanding of the function of complex, hierarchical biological systems will become possible, enabling advances in areas such as artificial photosynthesis, biocatalysis, and biopharmaceuticals

A major question in biological research is

> *Can the molecular basis of life's processes be understood to obtain a predictive understanding of the designs and mechanisms that underpin them?*

Obtaining this knowledge will make it possible to mimic the architectures and processes of living systems to create new bio-inspired materials and processes for developing new energy technologies. In addition, the information will provide insights into molecular and cellular processes that will enhance human health and quality of life.

For instance, nature uses sunlight to convert water into oxygen; most of the oxygen in the atmosphere is generated by plants, algae, and cyanobacteria through this reaction. Photosynthetic processes also convert atmospheric carbon dioxide (CO_2) into sugar. Understanding photosynthetic processes could open the way to the development of biomimetic processes to efficiently generate fuels and useful chemicals, such as photo-induced production of hydrogen or conversion of CO_2 to hydrocarbons.

Neutron scattering provides a number of advantages for the study of biological systems. First, neutrons are highly sensitive to hydrogen, so hydrogen atoms can be located and followed during biological processes to explore reaction pathways and chemical mechanisms. In addition, neutrons can readily distinguish hydrogen from its isotope deuterium, enabling a powerful experimental technique, isotopic contrast variation. Through the judicious substitution of deuterium for hydrogen, contrast can be increased or eliminated, making it possible either to highlight specific molecules or even parts of a living cell, or to make them invisible to neutrons. Finally, neutrons can probe delicate biological materials without damage.

As an example, for the case of the conversion of water into oxygen, the multi-subunit membrane protein photosystem II contains a small metal ion cluster, Mn_4CaO_5 (Fig. 6), that catalyzes the oxidation of H_2O, forming an oxygen-oxygen bond. This light-induced reaction is thought to involve five intermediate states (illustrated on the right side of Fig. 6). The oxidation state of the manganese atoms within the cluster alters during the reaction; and neutrons can probe both the structure and dynamics of the system during this critical process without interfering with it, unlike probes that can ionize the metal cluster. Further, with the new capabilities of the STS, it will be possible to obtain detailed insight into the water environment of the catalytic site. This information will provide critical information on light-induced changes in the hydrogen bonding network and protonation around the active site.

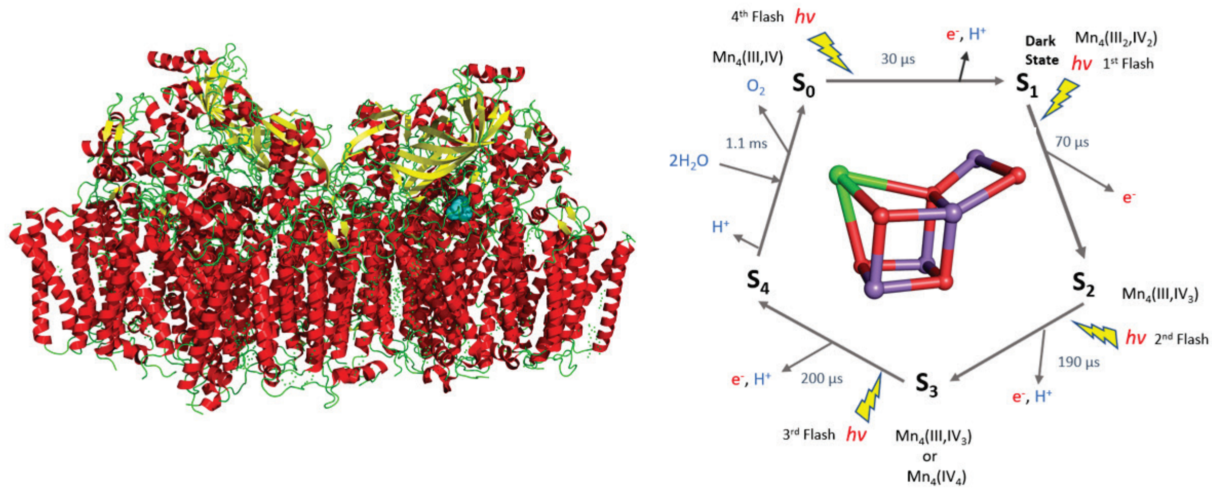

Fig. 6. Photosystem II and the Kok cycle. At left, the structure of the multisubunit photosystem II complex. At right, the classical Kok cycle with its five kinetic states (S_0 to S_4); a structural model of the oxygen-evolving cluster, an unusual metal cluster formed of manganese, calcium, and oxygen, is superimposed. The oxidation of H_2O is catalyzed via a series of light-induced transitions between the five kinetic states of the Kok cycle. *Image source: ORNL.*

The new capabilities of STS will enable researchers to rapidly take snapshots throughout the photosystem II reaction cycle and thus map the proton transfer pathways, providing critical insight into the full range of chemical mechanisms involved. This foundational information will accelerate the development of bio-inspired catalysts with impacts on areas ranging from fuel cells and solar cells to carbon capture technologies.

New scientific opportunities

The STS will dramatically extend the capabilities of neutron scattering for biological studies, revealing molecular events as they unfold over broad length and time scales. STS advances will enable the use of neutrons in a transformative way, integrating structural and dynamical descriptions of biological systems from the molecular to cellular levels. For instance, the dynamic assembly of many biological complexes involves networks of competing interactions, which constantly assemble and disassemble in response to their cellular environment. Gaining insight into these processes will provide researchers with opportunities to improve processes of importance to energy production, such as converting biomass to fuels and increasing drought resistance in crops, and processes key to human health, such as developing more effective treatments for diseases and producing bio-inspired materials for targeted drug delivery systems and biosensors.

The STS at SNS: Delivering World-Leading Neutron Science

The STS is designed to provide beams of cold neutrons with the world's highest peak brightness and will enable time-resolved measurements of chemical and physical processes, as well as simultaneous measurements of hierarchical architectures across unprecedented length scales, from the atomic scale to the micron and beyond. Technical advances that will be made to realize these world-leading capabilities and brief descriptions of the initial suite of eight instruments are presented below.

Enhanced Production of High-Energy Proton Pulses

A schematic layout of the SNS complex, including the proposed STS, is shown in Fig. 7. The linear accelerator (linac) produces pulses of negatively charged hydrogen (H^-) ions. The H^- ions are stripped of electrons to produce protons (H^+), which are subsequently "stacked" in the accumulator ring and delivered to the mercury target as a 1°μs pulse (reaching an intensity of 1.5×10^{14} protons per pulse) at a frequency of 60 Hz. The ongoing Proton Power Upgrade project will increase the power capability of the accelerator complex from 1.4 MW to 2.8 MW, which will enable the FTS and the STS to be operated simultaneously, yet independently.

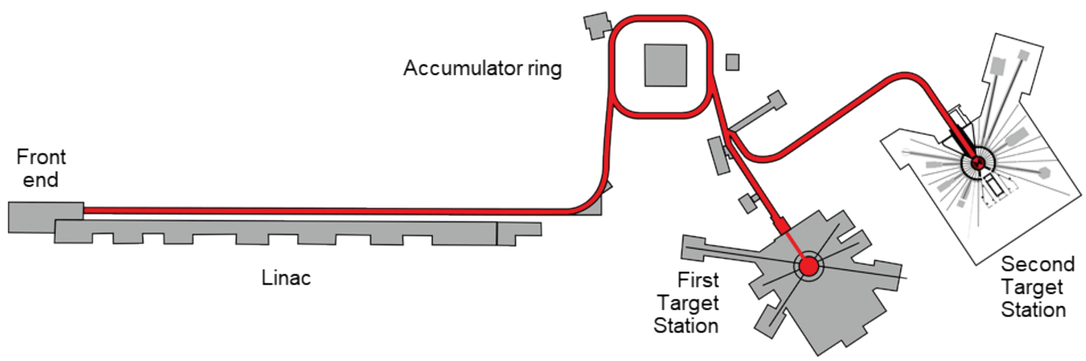

Fig. 7. Schematic layout of the SNS complex, including the proposed STS (at right). The beam path is shown in red. *Image source: ORNL.*

One of every four proton pulses produced by the accelerator complex and accumulator ring will be directed to the STS rotating tungsten target. STS will thus operate at 15 Hz with a proton beam power of 700 kW. The remaining pulses will be directed to the FTS mercury target, which will operate at 2 MW of proton beam power with 45 proton pulses delivered per second. These operating power and frequency parameters were selected to supply the FTS with its maximum design power of 2 MW to provide a world-leading intense source of thermal neutrons and to enable the STS to provide a world-leading intense source of cold neutrons with a broad range of wavelengths that can be used simultaneously.

These two target stations will provide complementary, world-leading capabilities for the US scientific community:

- FTS is optimized for production of pulsed beams of thermal neutrons with outstanding peak brightness that are ideal for studies of materials with structural measurements on the atomic scale and for fast dynamics studies of materials.

- STS will be optimized for production of pulsed beams of cold neutrons with world-leading peak brightness and a repetition rate of 15 Hz, providing broad energy/wavelength ranges that can be used simultaneously to examine materials and systems over broad length, energy, and time scales.

Compact Source Design for High Brightness

The STS neutron source will produce cold neutron beams of unprecedented peak brightness by employing three coupled processes. First, the incoming proton beam at the target will be compressed to a cross section of ~65 cm^2. Second, the water-cooled target, consisting of 21 segments of tungsten, will rotate at ~40 rpm to spread the power load. Finally, novel compact moderators will be designed to optimally couple to the target. This source design, coupled with a short proton pulse that produces neutrons in a short period of time, will result in world-leading cold neutron peak brightness (see Fig. 1). These innovations will provide the foundation for delivering the multiple orders-of-magnitude gains in instrument performance needed to address the science challenges envisioned for the STS.

Neutron Beamlines and Instrumentation

The STS will incorporate advances in neutron instrumentation and technologies that, coupled with the increase in neutron brightness, will enhance instrument performance by two orders of magnitude or more. These enhancements will enable scientific experiments that cannot now be conducted at any existing neutron facility worldwide. Advances in the technology that transports neutrons from the source to the sample position will enable fine control to provide smaller, focused beams with selectable angular divergence. These advances will be particularly important for the study of materials under extreme environments, such as high magnetic field, temperature, and pressure. Further advances in detector spatial resolution and maximum counting rates will also contribute to improved instrument performance. Finally, the STS will be complemented by new computational tools for data analysis and data mining as capabilities for quantitative comparisons to model predictions.

Table 1 presents brief descriptions of a preliminary set of instruments proposed for the STS. Specific design criteria, as well as the development of sample environments that will be constructed as part of the STS, will be defined by the user community.

Table 1. STS instrument concepts

Instrument	Capability	Features	Example studies
Small-angle Scattering	Perform time-resolved studies across a broad dynamic range of momentum transfer **Q**	High-speed statistical chopper to discriminate elastic from inelastic scattering and improve S/N; multiple detector arrays to collect data simultaneously over broad **Q** range	Time-resolved studies/ kinetics associated with materials synthesis, 3D printing, assembly of hierarchical polymer architectures, and formation of protein complexes
Simultaneous small-angle/wide-angle scattering	Bridge gap in length scales to simultaneously study the evolution of structure from subangstrom to ~300 nm	Three detector banks to provide continuous **Q** coverage; high-speed statistical chopper to discriminate elastic from inelastic scattering	Studies of soft matter under realistic processing conditions, crystallization processes from complex solutions (e.g., fracking and environmental wastes)
Reflectometry with horizontal sample surface	Perform real-time studies of changing interfaces, including free liquids	Two independent end stations with different neutron beam geometries to enable studies of liquid/gas and liquid/liquid interfaces	Studies of real-time changes at battery electrode/electrolyte interfaces, corrosion, and lipid membrane surfaces

Table 1. STS instrument concepts (continued)

Instrument	Capability	Features	Example studies
Chopper spectrometry	Measure weak signals intrinsic to low cross sections or small sample sizes with a wide range of incident neutron energies	Large detector solid-angle coverage approaching 2π sr, ability to use multiple incident energies in a single frame, polarized neutrons	Excitations in highly entangled systems (e.g., quantum spin liquids), out-of-equilibrium quantum dynamics, and artificial heterostructures
Combined indirect geometry spectroscopy/single crystal diffraction at high magnetic field	Determine structure and dynamics at extremes of magnetic field and low temperature	Dedicated magnet installation with fields up to 35 T, multiple analyzer arms capable of continuous **Q**-ω measurements	Magnetic structure/dynamics in field-induced normal state of superconductors; magnon spectrum in fully polarized, high-field state of frustrated magnetic materials
Small crystal diffractometer	Measure structures in small crystals (<0.01 mm^3 in volume with unit cell edges from 10 to 300 Å) in a single crystal orientation	High detector solid angle coverage (>5 sr), configurable and open end station enabling multiple sample environments, focusing mirror optics	Characterization of photosynthesis intermediates using pump-probe methods; mapping hydrogen positions in enzyme-catalyzed reactions
Diffractometry for magnetic structure studies	Elucidate magnetic local and long-range ordering in both powders and single crystals	Polarized neutrons, configurable neutron optics system to deliver high-intensity or high-resolution neutron beam, curved supermirror analyzer to provide full polarization	Polarized diffraction studies of complex topological structures in noncollinear magnetic systems
Combined diffraction, imaging, and small-angle neutron scattering	Perform multiscale studies of low-symmetry, complex structural materials	Novel detector enabling determination of full orientational distribution functions, selectable high-intensity or high-resolution modes	Observation of atomic and microstructural changes during phase transformations induced in materials; real-time structural studies in materials during processing and manufacturing

Conclusion

The proposed STS will provide wholly new capabilities that will substantially extend this nation's current resources for neutron scattering. Specifically, the STS is designed to produce the highest peak brightness of cold (long-wavelength) neutrons in the world, providing the US research community with transformative opportunities to study the structure, dynamics, properties, and reactions of complex materials that have heterogeneity, interfaces, and disorder, as well as conducting temporally resolved, in situ and operando studies of materials and associated chemical processes.

The design of the STS will enable studies of materials systems across larger length scales—from the atomic scale to the micron scale and beyond—revealing, for example, how polymeric materials self-assemble into hierarchical structures or molecules interact in living biological cells. These capabilities will be available to the broad research community, including academic, industrial, and government laboratories, as part of the DOE Office of Science User Facility program. The STS will incorporate major advances in neutron instrumentation and technologies to make optimal use of the high–peak-brightness cold neutrons produced by this new source. The STS will be a transformative new tool for addressing grand challenges in fundamental science and for developing materials for next-generation energy technologies, national security, and other national needs.

References

Banerjee, A.; Yan, J.-Q.; Knolle, J.; Bridges, C. A.; Stone, M. B.; Lumsden, M. D.; Mandrus, D. G.; Tennant, D. A.; Moessner, R.; Nagler, S. E. Neutron Scattering in the Proximate Quantum Spin Liquid α-$RuCl_3$. *Science* **2017,** *356,* 1055–1059.

BES Workshop Reports. Series of reports available at https://science.osti.gov/bes/Community-Resources/Reports (accessed September 2019).

Hemminger, J. C. (chair). *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science: A Report from the Basic Energy Sciences Advisory Committee,* U.S. Department of Energy, November 2015. Available at https://science.osti.gov/-/media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf (accessed September 4, 2019).

Srivastava, S.; Andreev, M.; Levi, A. E.; Goldfeld, D. J.; Mao, J.: Heller, W. T.: Prabhu, V. M.: de Pablo, J. J.; Tirrell, M. V. Gel Phase Formation in Dilute Triblock Copolyelectrolyte Complexes. *Nature Commun.* **2017,** *8,* 14131.

Zhan, C.; Lian, C.; Zhang, Y.; Thompson, M. W.; Xie, Y.; Wu, J.; Kent, P. R. C.; Cummings, P. T.; Jiang, D.; Wesolowski, D. J. Computational Insights into Materials and Interfaces for Capacitive Energy Storage. *Adv. Sci.* **2017,** *4,* 1700059.