Spallation Neutron Source Second Target Station Project (SNS-STS)

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Spallation Neutron Source Second Target Station

Executive Summary

The proposed Spallation Neutron Source (SNS) upgrade will provide the United States with a world-leading fourth generation neutron source that enables researchers to address emerging grand challenges of central importance to the mission of the Department of Energy (DOE). The upgrade comprises two major activities: a proton power upgrade of the existing accelerator structure (SNS-PPU), which provides a platform for the construction of a second target station (STS) complex with an initial suite of beam lines (SNS-STS). SNS-STS is described in this document whereas SNS-PPU is described in a companion document *Spallation Neutron Source Proton Power Upgrade*. This STS upgrade was recognized as being "absolutely central" to US science in the 2013 Basic Energy Sciences Advisory Committee (BESAC) facilities prioritization review.[1] STS is vital to future competitiveness of US science and technology and will ensure US leadership in neutron scattering even with the advent of game changing science capabilities promised by upcoming sources, such as the European Spallation Source (ESS) now under construction in Sweden. Oak Ridge National Laboratory (ORNL) has resolved the "science/engineering challenges" identified in the 2013 BESAC prioritization review in *Instruments for Emerging Science: A Science Case for the Second Target Station* and *Technical Design Report Second Target Station*.[2] ORNL is now ready to proceed to construction of SNS-PPU and SNS-STS, and to deliver ground-breaking new scientific capabilities to realize the transformative opportunities identified in the 2015 Basic Energy Sciences' (BES) Grand Challenges update.[3]

The companion document, *Spallation Neutron Source Proton Power Upgrade,* describes the SNS-PPU project, actions being taken to achieve the SNS first target station's (FTS) design envelope, and scientific productivity impact and growth. This document describes the compelling science case for the SNS upgrade, and outlines the elements of the SNS-STS project. The mission need and science case for SNS-STS and SNS-PPU are the same. ORNL has explored directly the areas and challenges where neutrons will play a vital role in the future of US science at a series of workshops. The workshop attendees focused on defining compelling scientific and technological challenges for the decade ahead that are inaccessible to other techniques or where the contribution of neutrons in combination with other techniques is vital. The panelists from all workshops concluded that in the areas of science covered, neutrons play a unique and strong role in understanding structure and dynamics in materials required to develop future technologies. They determined that world-leading neutron facilities, such as the STS, will be needed to complement other forefront advanced research user facilities in addressing the DOE mission. They specifically noted that complementing the strengths of the High Flux Isotope Reactor (HFIR) and SNS-FTS with the STS meets the US needs for more intense neutron beams in the long-wavelength (cold) regime and for instrumentation that can sample a broad dynamic range in length and time scales. The proposed SNS-PPU and SNS-STS upgrades will enable the SNS to reach its full potential as a world-leading fourth generation source with increased neutron flux on available beam lines on FTS, and with a STS supporting 22 additional beam lines with transformative new scientific capabilities.

Science Needs and Emerging Challenges

In parallel with the assessment of progress on BES's Grand Challenges launched in 2014, ORNL explored directly the areas and challenges where neutrons will play a vital role in the future of US science. This complementary assessment was made at four workshops on the future of quantum condensed matter, soft matter, biology, and the frontiers in materials discovery that engaged science leaders in these areas. The areas encompass and directly map to the transformative opportunities identified in the BES Grand Challenges update. Quantum materials maps most directly to **harnessing coherence in light and matter**, while soft matter and biology are aligned primarily with **mastering hierarchical architectures and beyond-equilibrium matter,** and frontiers in materials discovery explored many of the topics in **beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces, and disorder.**

The workshop attendees focused on defining compelling scientific and technological challenges for the decade ahead that are inaccessible to other techniques, or where the contribution of neutrons in combination with other techniques is vital. They also identified areas where a step change in capabilities is needed. Panelists from all four of the workshops concluded that the addition of STS to ORNL's existing neutron sources (HFIR and SNS-FTS) makes it possible to meet these challenges. They specifically noted that complementing the strengths of HFIR and SNS-FTS, SNS-STS meets the US needs for more intense neutron beams in the long-wavelength (cold) regime and for instrumentation that can sample a broad dynamic range in length and time scales. Examples of science challenges from each of these workshops are outlined below (See Fig. 1 of *Spallation Neutron Source Proton Power Upgrade* for illustrative examples).

Grand Challenges in Quantum Materials.[4] Although normally associated with physics at the atomic scale, quantum coherence can give rise to spectacular properties when it transcends that scale through a rich variety of collective behaviors in so-called quantum materials. Neutrons provide access to the spatial and temporal electronic correlations and have played a pivotal role in the rapidly developing understanding of these materials. They have proved indispensable for addressing a number of crucial problems from understanding the exotic ground states that emerge in quantum spin systems, quantum critical phenomena, topological states of matter, and quantum materials out of equilibrium, to the physics underlying unconventional superconductors and itinerant magnets. The workshop panelists were confident that the advanced capabilities of the STS for probing structure and dynamics in thin films/heterostructures/nanomaterials will be invaluable for developing new devices and spintronics, batteries and other technologies. They also concluded that STS will directly address the increasing importance of mesoscale phenomena for controlling properties, a major trend in the coming years. The ability to realize orders of magnitude in gains at the STS can be anticipated to have vast impact on understanding of quantum materials and their application to future technologies, by giving direct information on quantum coherence and dynamics. With new science comes new challenges. For example, phenomena in mesoscale and complex matter can occur on length and time scales that are not optimally sampled by existing sources and associated instrumentation**.** In the case of topological quantum materials, these phenomena can have quite different signatures from any encountered before and involve both nanoscale and mesoscale features in new ways.

Grand Challenges in Soft Matter.[5] Soft matter (including polymers, surfactants, nanoparticles, gels, etc.) provides almost endless complexity and tunability for the design of materials with specific functionalities. These materials are the quintessential hierarchical system in that their macroscopic properties arise through a combination of interactions over several length and time scales from the nanoscale of individual building blocks to the microscale of long chains and self-assembled systems. Their properties can also be controlled by interfaces, transport, and environment. The widespread impact of soft matter technologies will require looking at soft matter under industrial processing conditions, understanding active soft materials, expanding our ability to make quantitative measurements, and gaining insight into the effects of poly-dispersity. The workshop panelists concluded that while neutrons are an essential tool for studying soft matter today, STS will provide a high flux of long wavelength neutrons over a wide bandwidth ideally suited to simultaneously studying multiple temporal and spatial scales, which are crucial to understanding complexity in soft and hierarchical systems as well as monitoring their assembly, out-of-equilibrium behaviors, and function *in operando*.

Grand Challenges in Biology.[6] Despite the advantages in using neutrons for the study of biological matter, significant technical gaps must be closed, including the low flux and limited dynamic range of currently available beams of cold neutrons. STS will bridge those gaps and contribute towards gaining a predictive understanding of the behavior of complex biological systems, one of the greatest scientific challenges that researchers face over the next decade. This understanding will guide in protecting and repairing physiological systems; it will allow mimicking of the architectures and processes of living systems to create new biomaterials and bio-inspired technologies; and it will provide the information necessary to manipulate micro-organisms and their ecosystems to create new biotechnology and biorefinery solutions to emerging energy and environmental challenges. A defining feature of STS is its integrated use of new techniques to manipulate spins in neutrons, electrons, and nuclei. This allows new types of experiments that can realize new science. An example of this is dynamical nuclear polarization where nuclear spins can be coherently manipulated using Nuclear Magnetic Resonance (NMR)-type techniques. Application of spin manipulation techniques to hydrogen promise hundred-fold gains above and beyond the higher instrument performance of STS, and could revolutionize our understanding of hydrogen and water in structural biology.[7]

Fig. 1. Unique features of STS.

The workshop participants agreed that STS will enable the use of neutrons to be used in a transformative way to unify the structural and dynamical description of biological systems across relevant length and time scales, by providing intense beams of cold neutrons and a suite of neutron instruments which simultaneously survey broad ranges of length and time. They also concluded that in combination, these advances integrated with the development of computational tools and complementary techniques will transition the concept of a predictive understanding of biological systems to a reality.

Grand Challenges in Materials Discovery, Characterization, and Application.[8] Predictive modeling of materials holds the promise of accelerating the development of a new generation of energy technologies; however, as a prerequisite, this development requires an understanding of materials' hierarchical and heterogeneous structure and dynamics from the atomic scale to real-world components and systems.[9] In addition, understanding and controlling non-equilibrium processes will be critical to achieve efficient synthesis approaches to realize these revolutionary materials. The workshop panelists observed that the unique physical properties of neutrons make high-intensity beams indispensable to materials discovery, characterization, and application, complementing the capabilities of electrons and photons. For example, the ability of neutrons to penetrate chambers will allow chemical reactions and processes associated with catalysis and separations to be monitored and understood under realistic conditions. Neutron spectroscopy, because it is not limited by optical selection rules, can also provide additional information on chemical reactions not accessible to other analytical spectroscopic techniques. They also noted that neutrons are important for understanding the role of disorder and defects in determining the properties of materials; addressing the fundamental challenges of glasses and liquids, as well as fluid flow and reactivity; conducting in situ studies (including under pumping conditions), kinetics studies, explorations of materials growth and synthesis, and explorations of materials under extreme condition; and understanding how components and integrated materials in devices function under realistic conditions using instruments that can combine multiple techniques such as imaging, diffraction and spectroscopy.

Fig. 2. Transformative science capabilities that will be enabled at STS.

In the case of real-life materials, the combination of very extensive dynamic range in space and time and ability to simultaneously integrate multiple characterization techniques will open up access to many of the most important classes of advanced materials (i.e. complex and hierarchical materials): it can also be used to follow the impact of defects and processing from atomic to real-world scales. Moving beyond current neutron sources, STS provides the performance to monitor out-of-equilibrium behavior and kinetics whilst simultaneously capturing all relevant scales.

Integrated understanding of synthesis and processing represents a frontier beyond the prediction of materials properties. The challenge of tracking rapid changes at multiple length-scales requires a new kind of powerful instrumentation as envisaged at STS that incorporates multiple modalities (e.g. X-rays, NMR and neutrons), and the ability to combine sophisticated synthesis and processing apparatus with highly configurable instrument layouts and tunable optics. A new emphasis for the STS is on designing a beam line as a laboratory. From real-time chemistry to new horizons in matter under extreme conditions the power and adaptability of the STS beam lines will allow a step change in the ability to conduct complex experiments in situ. For example, STS instruments will probe dynamics in materials at 100 GPa pressures that have been inaccessible to date but where unique insight lies, or at the highest magnetic fields that have so far only been available at dedicated magnet laboratories.

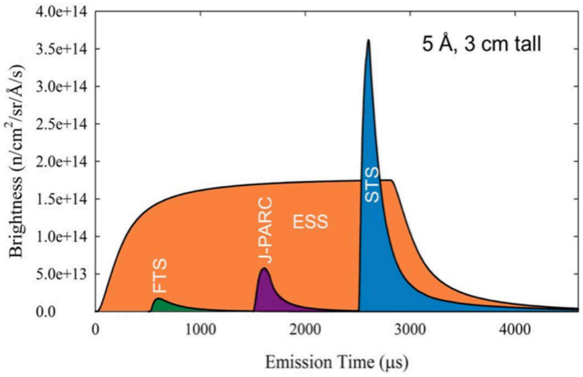

Fig. 3. Neutron pulse shapes for existing and planned neutrons sources with coupled cryogenic moderators. Pulse shapes have been displaced along the x-axis for clarity.

The transformative opportunities of neutrons and imaging will be realized with advanced optics and STS beam intensities combining to map space, time, and wavelength in small volumes to understand complex textures and inhomogeneities that control the transport and strength in energy materials. High-throughput and automated beam lines are needed to provide rapid screening and characterization of materials supporting the scale of future synthesis efforts. Advanced materials are essential to address a number of societal needs particularly in energy and the ability to rapidly characterize them is essential to accelerate their discovery and application. High-throughput instrumentation can provide crucial data on synthesis bottlenecks and optimization conditions and insight into processing.

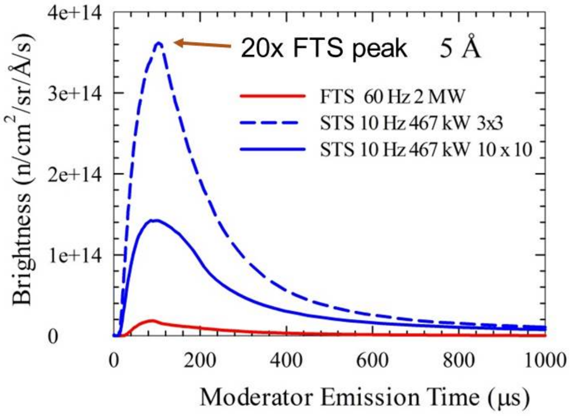

Fig. 4. Neutron pulse shapes at 5 Å from the coupled para-hydrogen moderator of FTS and STS.

A common theme that emerged from all four workshops is that beyond any other factor, science at STS will be defined by the opportunities in high-performance computing (HPC) and data. Only with these advances is it becoming possible to create and utilize the very large multimodal and multi-technique data sets that STS will produce. The development of HPC capabilities will enable the combination of data sets including unified reconstructions of scattering and imaging data. Movies, derived from simultaneous measurement of complex systems with (e.g.) NMR, X-rays, bulk probes, etc., are needed to understand the interactions of components and the influence of varying starting conditions and stimuli. STS provides the opportunity to create instrumentation for addressing such challenges with high-quality neutron data as an anchor point. Finally, neutrons characterize phenomena on length and time scales that are well matched to computational modeling making them indispensable for verifying methodologies and predictions for materials by design.

In summary, the scientists from all four workshops noted that in each of the four science areas covered, neutrons play a unique and strong role in understanding structure and dynamics in materials required to develop future technologies. They concluded that world-leading neutron facilities, such as the STS, will be needed to complement other forefront advanced research user facilities in addressing the mission of DOE. To meet the needs outlined at the four workshops, a study was undertaken to further identify current neutron scattering capability gaps and source and instrument concepts that could close those gaps. A report from that study outlines 22 instrument concepts each capable of delivering unprecedented levels of performance.[10] The report also presents a compelling science case for the STS. The unique capabilities of the STS, illustrated in Fig. 1, will be combined with innovative instrument and source technologies in truly new ways to attain the very large gains in performance and transformative science capabilities, illustrated in Fig. 2.

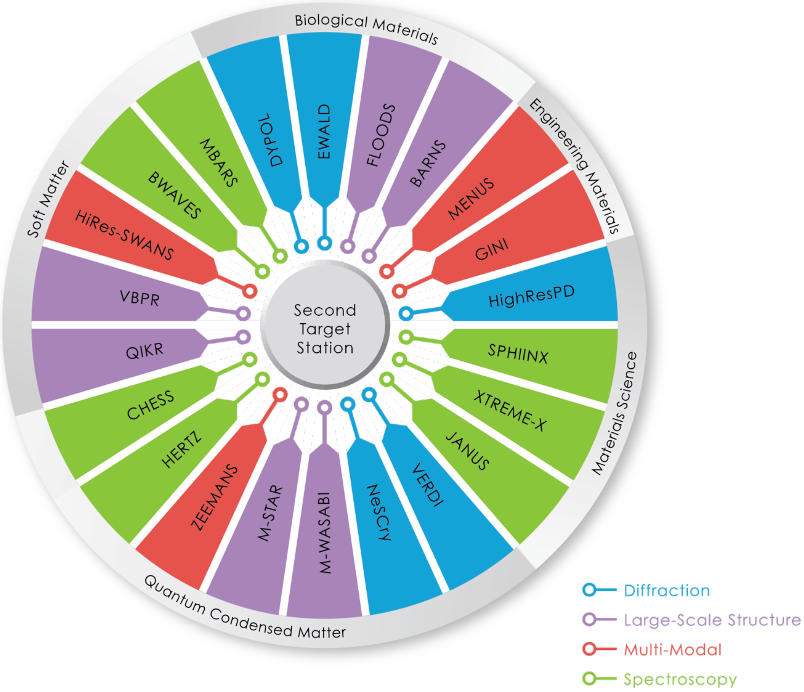

Fig. 5. Twenty-two instrument concepts were discussed during the STS user workshop, four of which are described in Fig. 7 to 10.

Enabling Grand Challenge Science with the Second Target Station

A high-brightness pulsed source optimized for cold neutron production operating at 10Hz[i] in conjunction with innovative instrumentation has been shown to be the most effective way to address the capability gaps of current neutron sources, as identified by panelists in the four workshops discussed above.[11] STS will use one out of every six proton pulses produced by the SNS accelerator complex to produce cold neutron beams with the highest peak brilliance of any current or projected neutron source worldwide (see Fig. 3). A proton beam power of 467 kW will be diverted to the new complex and its solid tungsten target. The three moderators located above and below the target will feed up to 22 experimental beam lines with neutron energies conditioned to their needs. The exploitation of compact source/moderator technology is key to delivering the highest brilliance cold neutron beams, and in combination with new instrumentation will allow STS to address hierarchical materials, out-of-equilibrium matter, quantum materials and devices, and heterogeneous and real life materials, beyond the ability of any existing source.

Elements of the SNS-STS Project

The technical design report (TDR) provides a detailed description of the proposed STS project.[12] The design work leverages the extensive expertise gained from construction of FTS and its instruments, as well as 10 years of accumulated operational experience. A number of innovations directly leading from this knowledge base have been incorporated, resulting in simplification, cost savings and improved performance. These include elimination of massive beam line shutters, which greatly improves neutron transport to instruments; adoption of a solid tungsten target creating a compact neutron production zone; extensive adoption of standardization of instrument components; and early establishment of building technical requirements. The preliminary cost estimate assuming 30% contingency and escalation is $1,327 million. The project is divided into four major subsystems, described below.

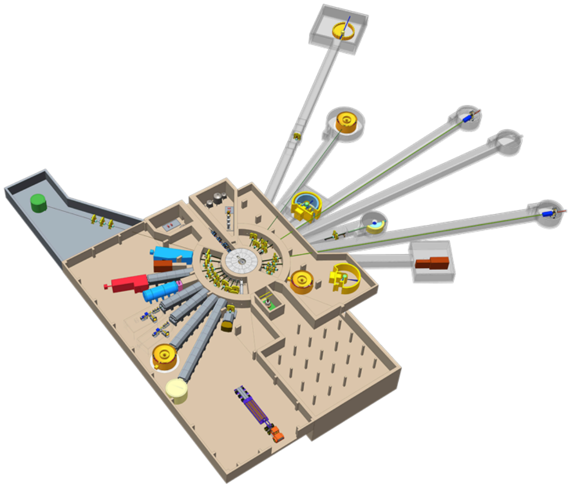

Fig. 6. Proposed layout for STS instruments.

Conventional Facilities[ii]

The STS complex will be located in unoccupied space east of the existing SNS-FTS. The project includes approximately 380,000 ft^2 of new buildings making conventional construction a major contributor to project costs. The layout consolidates instruments with beam lines less than 40 m long in a hall adjacent to the STS target building freeing up space for the longest beam lines on the opposite side of the STS target. Beam lines as long as 120 m (50% longer than the longest FTS beam line) can be accommodated with this layout. Relative to FTS, the footprint of the expensive target building is greatly reduced minimizing its cost while greater flexibility is preserved in specifying requirements for instrument buildings.

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[i] Operation at 10 Hz is required (as compared to FTS at 60 Hz) to provide the large time-of-flight intervals corresponding to the broad time and distance scales required to characterize complex materials.

[ii] The scope for conventional facilities includes site improvements, buildings, accelerator tunnels, cooling systems, plant-wide control systems, waste handling systems, maintenance systems, fire protection systems, and all other services required to support the accelerator, target and neutron instruments.

Neutron Target and Moderators[iii]

Coupling a compact neutron production zone to an optimized moderator geometry is the key to producing the high peak brilliance neutron beams that will be the signature feature of the STS. An optimally sized 30 cm^2 proton beam strikes a 1.1 m diam. rotating solid tungsten target. The beam is concentrated into one-fifth the area of FTS and produces a very high density of neutrons illuminating a matching small-volume moderator system. The choice of tungsten moves the peak neutron production zone forward matching the moderator requirements and improving performance. Developments in cold neutron moderator technology show geometric optimizations gaining factors of 2 to 3.[13] Taken together, this will produce a peak brightness for cold neutrons at least 20 times that of FTS as shown in Fig. 4.

Accelerator Systems[iv]

The project will provide the infrastructure to divert every sixth proton pulse away from FTS. The beam will be diverted (after compression in the Ring) to a new line feeding the STS by a series of kicker magnets inserted in the existing Ring to Target line. Additional magnets will further deflect the beam into the transport line to the new target. A final set of quadrupole magnets will tailor proton beam shape and distribution to match the compact source design. The key design requirement is to flatten the proton beam distribution across a small beam profile at the neutron target supporting the STS compact neutron source concept.

Instruments

At the first STS user workshop held at ORNL, October 27-29, 2015, more than 200 researchers discussed the science that could be addressed by STS.[14] They considered 22 instrument concepts, each capable of delivering unprecedented levels of performance (Fig. 5 and 6). These offer multimodal measurements both in terms of using advanced optics and computing to allow measurement and integration of multiple types of neutron measurement simultaneously, but also enabling orthogonal, complementary techniques to monitor the system in parallel. In addition, the flexibility of design offered by new manufacturing technologies and complex data handling will allow the concept of a laboratory on a beam line to be realized where steering of complex interactive experiments is made in real time, and in situ/in operando conditions can be designed as an integral part of the beam line from the beginning of operation. Users selected 12 instrument concepts as top priorities for further development as part of the effort in assembling the STS Conceptual Design Report (CDR). Four examples of selected instrument concepts are shown in Figs 7, 8, 9, and 10. ORNL will continue to engage the science community over new instrument concepts and compelling science questions throughout the duration of the project resulting in the final selection of the initial eight beam lines that will be built at the STS.

[iii] Proton beam reaches the target horizontally producing neutrons that feed three “wing” moderators located above and below. Two moderators will be cold, coupled para-hydrogen placed in the favored positions in order to produce the highest cold neutron flux. The third de-coupled, multi-spectral moderator will be optimized to produce sharp neutron pulses.

[iv] The Spallation Neutron Source Proton Power Upgrade (SNS-PPU) seeks to double the current SNS accelerator beam power, with 2 MW available for FTS and appropriate margin available for operation of both FTS and STS.

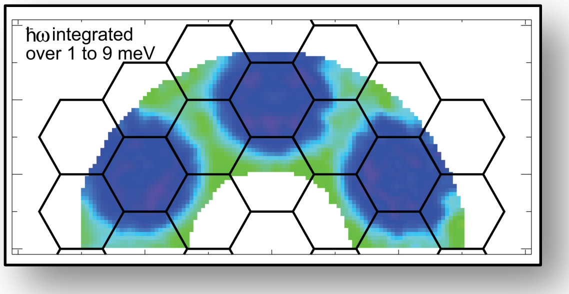

Fig. 7. ZEEMANS will access new regimes in quantum materials such as quantum spin liquids. ZEEMANS is a next generation instrument concept that integrates the extreme sample environment of high magnetic field with a suite of neutron experimental techniques on a single beam line. This instrument will exploit the laboratory on a beam line concept because it will be reconfigurable over a full range of polarized or non-polarized neutron spectroscopy, diffraction, reflectometry, and small angle scattering options. Further, multimodal measurements and sample manipulations will be possible with NMR and bulk probes. Measurements on ZEEMANS will be over an order of magnitude faster than possible with existing instruments. The high peak brightness of the STS makes possible the small samples volumes required to access the most extreme conditions. The broad dynamic range of the STS allows simultaneously access to the length and time scales that characterize the complex materials of interest. ZEEMANS will have major impact across the whole range of materials based sciences enabling ground breaking experiments. However, its greatest impact will be in defining the frontier in high magnetic field neutron scattering, creating no less than the world center for high magnetic field neutron scattering at ORNL. A > 35 T magnetic system will provide access to previously inaccessible phenomena in matter. Image credit: NIST, http://www.nist.gov/ncnr/spin-121912.cfm

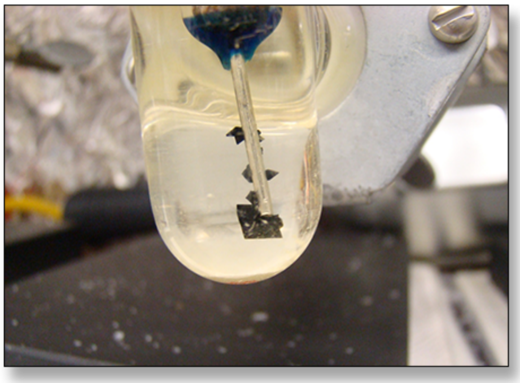

Fig. 8. CHESS will allow the first inelastic neutron measurements of collective phenomena in the tiny available crystals of organic superconductors. CHESS is a next-generation cold neutron chopper spectrometer that will have over two orders of magnitude gains in performance relative to existing instruments. The spectrometer will take full advantage of the increased peak brilliance of the STS to focus neutrons onto very small samples opening the technique to a broader range of quantum and functional materials. The broad dynamic range of the STS allows each of the 10 Hz pulses to be divided into 4 to 10 sub-pulses using an innovative new technique called repetition rate multiplication. This will maximize the range of energy and momentum transfers that can be simultaneously surveyed enabling new measurements in materials with excitations over broad ranges of energy. CHESS will include full three-dimensional polarization analysis to enable separate measurements of multiple components of the $S_{ab}(Q, \omega)$ tensor.

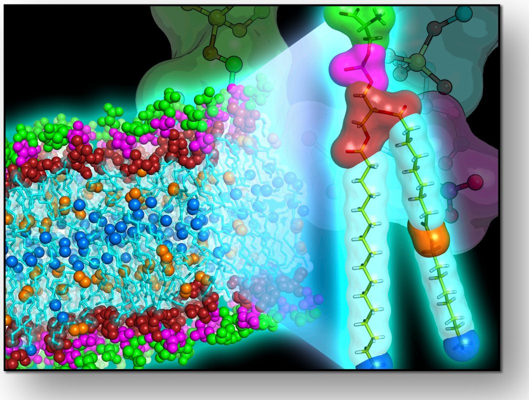

Fig. 9. QIKR will characterize kinetic pathways of multicomponent hierarchical assembly in soft materials. QIKR is a next generation neutron reflectometer that will have over two orders of magnitude gains in performance compared to existing instruments. Additional gains may be anticipated by incorporating recent advances in neutron optics design using elliptical or parabolic focusing onto the sample. Importantly, the high peak brightness and broad dynamic range of STS will enable a full decade in momentum transfer Q (e.g. $0.02\ \text{Å}^{-1} < Q < 0.2\ \text{Å}^{-1}$) in a single setting. This will permit users to simultaneously probe thin film compositional profiles and surface roughness from tens to tenths of a nanometer in seconds or less. QIKR will therefore open new scientific possibilities for structural and kinetic studies of hierarchical and heterogeneous systems at solid, solid/liquid and free liquid surfaces and interfaces.

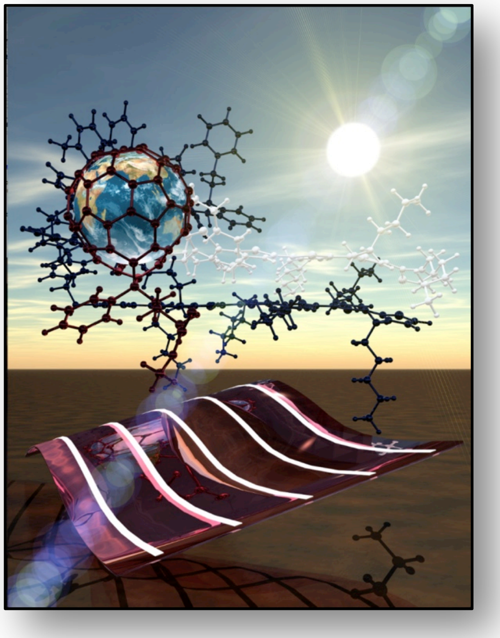

Fig. 10. HiRes-SWANS will resolve nanoscale features in newly developed complex, disordered materials in which local ordering is equally critical for material performance, as is commonplace in the soft matter sciences. The instrument will fill the capability gap that exists between high-resolution diffractometers at SNS and small-angle neutron scattering instruments at HFIR. Specifically, photovoltaic materials, polymer-nanomaterial composites, superhydrophobic materials, and biomaterials have properties that arise from interplay between nanoscale and molecular structures. The **HiRes-SWANS** combines features of a high-resolution neutron diffractometer with the ability of a small-angle neutron scattering instrument to probe length scales spanning from the interatomic out to tens of nanometers simultaneously. The combination of broad dynamic range ($0.01\ \text{Å}^{-1} < Q < 6\ \text{Å}^{-1}$), high Q resolution ($\Delta Q/Q < 1\%$) and grazing-incidence scattering capabilities that could be achieved on a beam line at the high-flux, low repetition rate STS, a truly unique instrument optimized for studying many of the newly developed, novel materials with technological game-changing potential can be studied as has never been capable previously.

Summary

In conclusion, the STS represents a step change in neutron capabilities that connects directly with the transformational science needed for the future. It was recognized as being "absolutely central" to US science by BESAC in the 2013 facilities prioritization review.[15] It is vital to future US science technology, and will ensure US leadership in neutron scattering even with the advent of game changing science capabilities promised by upcoming sources such as the ESS. ORNL has resolved the "science/engineering challenges" identified in the BESAC review as described in *Instruments for Emerging Science: A Science Case for the Second Target Station* and *Technical Design Report Second Target Station*.[16] ORNL has established a STS Project Planning Office to prepare the project management structure to deliver a CDR for the SNS-PPU and the STS for CD-1 review as early as 2018, in anticipation of potential funding. A core set of design engineers, physicists, and project control specialists support this effort, largely matrixed from the operational organization. The staff has experience with operation of the SNS accelerator, target and instrument systems, and importantly key team personnel with experience from the original SNS construction project. Having addressed all issues, ORNL is now ready to proceed to construction of SNS-PPU and SNS-STS and to deliver ground-breaking new scientific capabilities to realize the Transformative Opportunities identified in the BES Grand Challenges update.

Note: These references are available in pdf format at this website: https://conference.sns.gov/event/21/

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