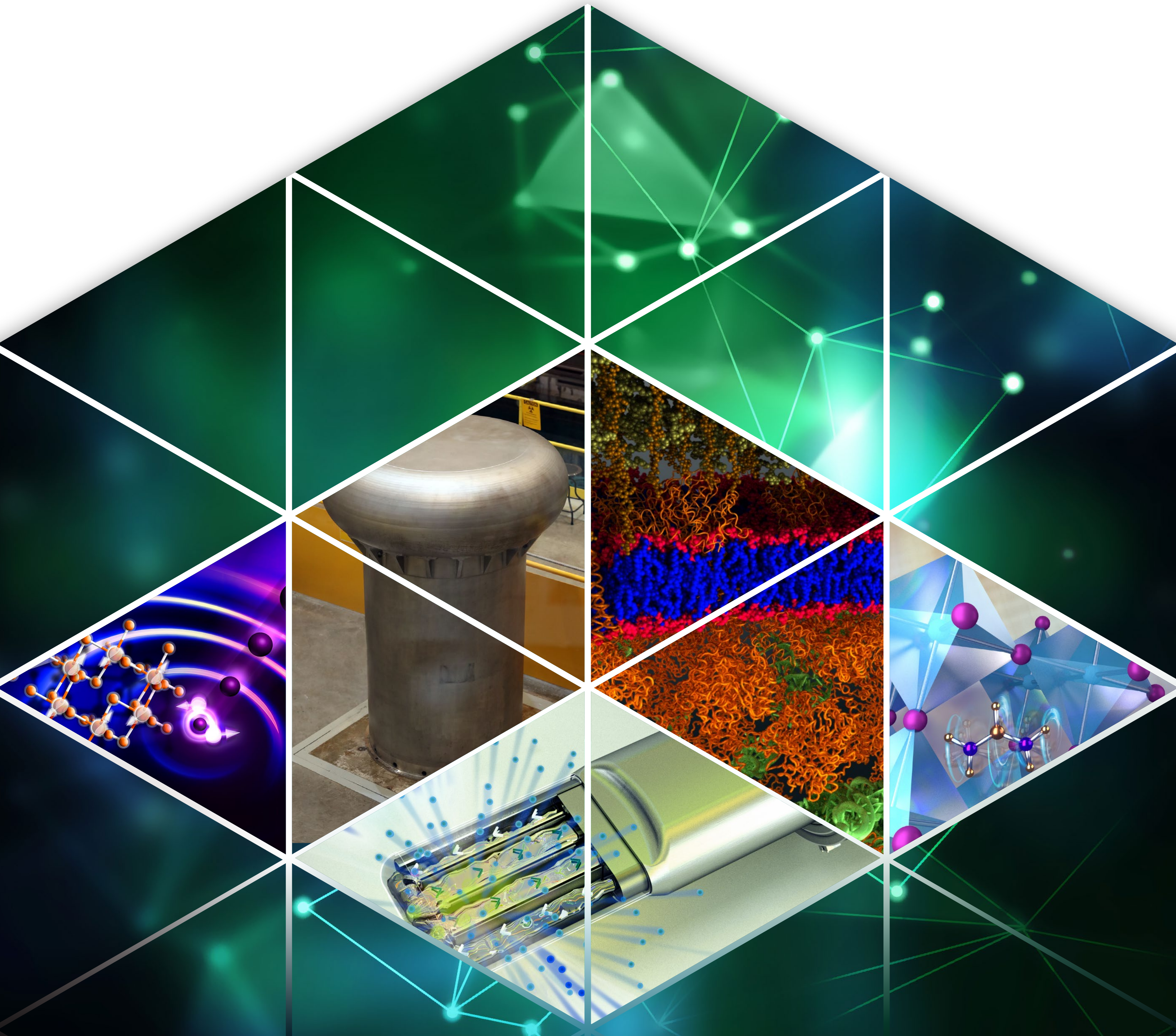
2019 Oak Ridge National Laboratory

Neutron Sciences Annual Plan



OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

U.S. DEPARTMENT OF ENERGY | Office of Science

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2019 Oak Ridge National Laboratory
Neutron Sciences Annual Plan

Introduction

The scientific breakthroughs that transform our future are accelerated by the availability of advanced research user facilities. The U.S. Department of Energy (DOE) Office of Basic Energy Science (BES) maintains several user facilities as national resources that allow researchers, including those from universities, national laboratories, research institutes, and industry, to conduct experiments that would be impossible to conduct at their home institutions. Among these, the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) operated by Oak Ridge National Laboratory's (ORNL) Neutron Sciences Directorate (NScD) provide neutron scattering capabilities which have enabled researchers to make scientific discoveries that would not have been possible using any other technique. (Fig. 1) Our vision is to be the world's leading provider of neutron science and technologies, enabling scientific discoveries and solving scientific challenges that can be best addressed using neutrons. We are proud of our progress towards higher power, higher reliability, and higher science impact at SNS and HFIR over the past few years.

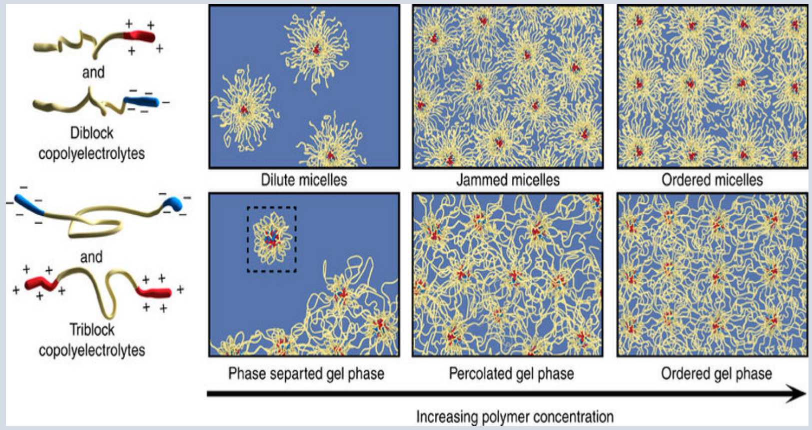
NScD has the mission of advancing the science of neutron scattering in support of the greater scientific community. To achieve this mission, NScD will (1) improve and optimize its existing neutron scattering facilities on a continuous basis, (2) develop innovative neutron scattering methods, sample environments, and technologies, (3) sustain and improve neutron production at SNS and HFIR, and (4) take advantage of core capabilities and expertise found across ORNL. Achieving these goals will require improving neutron sources, instruments, and methods.

This document summarizes major FY 2018 achievements and outlines actions for FY 2019 that are designed to continue to move us towards achieving our vision. At the beginning of FY 2019, six new organizational goals were set for the next three-five years.

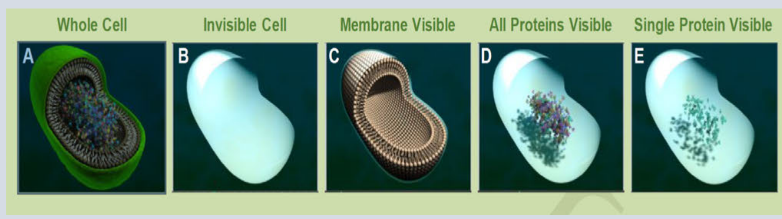
- Greater scientific productivity and impact, with > 500 instrument publications per year
- Reliable operations of HFIR at seven cycles per year and SNS at 1.4 MW
- New instruments, with VENUS constructed by 2022
- Complete HFIR-life extension and upgrade outage by 2024
- Accelerator research and development providing a 2.8 MW capable SNS by 2024
- Ready for Critical Decision (CD)-1 of Second Target Station (STS) by 2019

SNS and HFIR scientific discoveries that depend on neutrons…

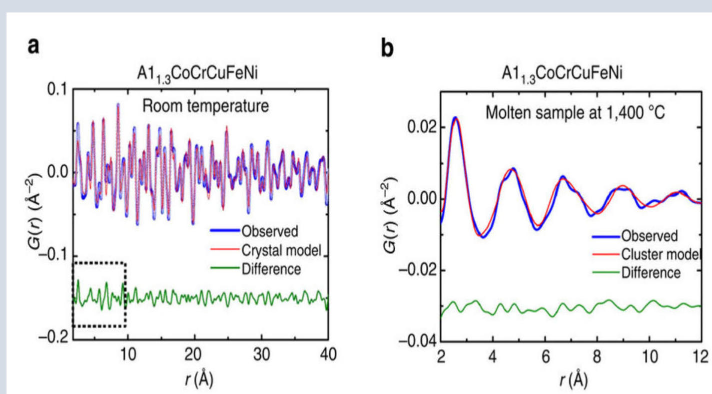
Soft Materials The sensitivity of neutrons to hydrogen, the possibility of selective deuteration, and their high penetrating and non-destructive nature were used in scattering studies of the assembly of functionalized polyelectrolytes. Diblock polymers assemble into star-like micelles. At low polymer concentration, discrete micelles remain suspended in the solution. With increasing polymer concentration, micelles jam, thus forming viscoelastic solids, and eventually order in cubic lattice structures. Triblock polymers are expected to form flower-like micelles at extremely low concentrations, but instead form gels that phase separate from the solution. This discovery raises the prospects for gels with applications in tissue engineering, agriculture, water purification and theranostics (Srivastava et al. *Nature Communications*, 2017).



Living Systems The above properties of neutrons are also ideal for studying biological complexes or pathways *within living systems*. A further advantage for using neutrons is the ability to combine H_2O/D_2O contrast variation with specific deuteration to sequentially highlight different components of these systems. For instance, a selectively labeled protein subunit called GroEL was expressed in a culture of living bacterial cells as quasi-elastic neutron scattering revealed important differences in its dynamic behavior within the crowded cytosolic environment compared to *in vitro*. These subunits form a complex that is essential for protein folding and defects in their behavior are associated with numerous diseases (Anunciado et al. *J. Physical Chemistry Letters*, 8, 1899, 2017).

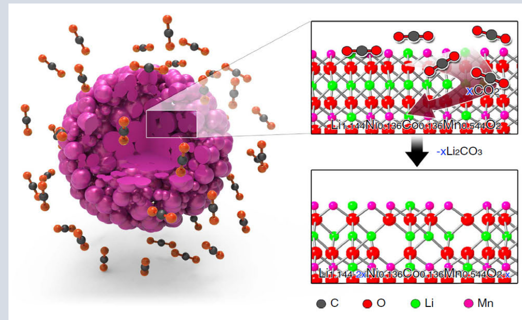


Advanced Alloys High entropy alloys comprise a new class of materials with exceptional properties, such as formability, electrical conductivity, oxidation resistance, and high temperature strength, which are currently attracting significant attention. The high penetration and the different sensitivity of neutrons to metals with similar atomic number was used in total scattering experiments to reveal information about a phase transitions from an order room temperature phase a) to a high temperature molten phase b), in one alloy ($Al_{1.3}CoCrCuFeNi$) that will drive its further development by tuning its composition (Santodonato et al. *Nature communications,* 6, 5964, 2015).

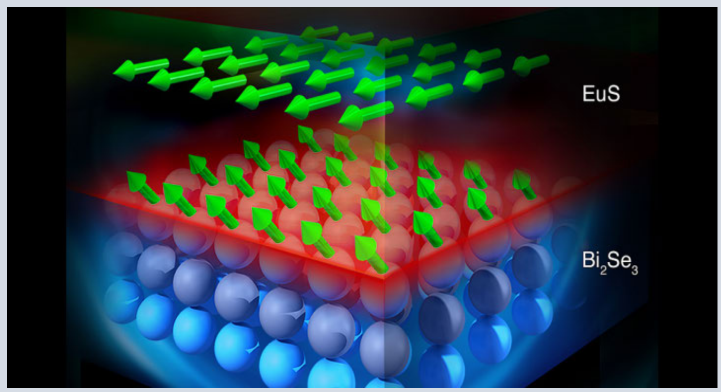


…SNS and HFIR scientific discoveries that depend on neutrons

Improved Batteries The high penetration and high sensitivity of neutrons to small mobile cations, such as hydrogen, lithium, and sodium make them a unique probe for obtaining new insights into the operation of batteries. A neutron diffraction study shed light on how changing the oxygen composition of a lithium-rich cathode material could improve battery performance, particularly in high-energy applications such as electric vehicles. By reducing oxygen release during its charging cycle this approach also reduces the flammability of the battery (Qiu et al. *Nature Communications,* 2016).



Topological Insulators A unique property of topological insulators is that electrons can flow on the surface without dissipation, while the bulk of the material serves as an electrical insulator. However, to realize devices based on this property magnetism can be introduced by interfacing the topological insulator with a layer of ferromagnetic insulating film without disturbing the bulk insulating properties. The sensitivity of neutrons to magnetism and their innate ability to pass through materials in a nondestructive fashion was used in a polarized neutron reflectometry study to detect such a hidden magnetic signal. The discovery promises new opportunities for next-generation electronic and spintronic devices such as improved transistors and quantum computing technologies (Katmis et al. *Nature*, 533, 513, 2016).



Quantum Spin Liquids A quantum spin liquid is a state of matter characterized by the entanglement of particles over distances that are long compared to the atomic scale, and holds promise for future applications in quantum computing and electronics. The sensitivity of neutrons to magnetism was used in an inelastic neutron scattering study to reveal a continuum of magnetic excitations, a key signature of the quantum spin liquid state, in a rare earth–based metal oxide ($YbMgGaO_4$) providing new information on microscopic interactions in this material (Paddison et al. *Nature Physics*, 13, 117, 2016).

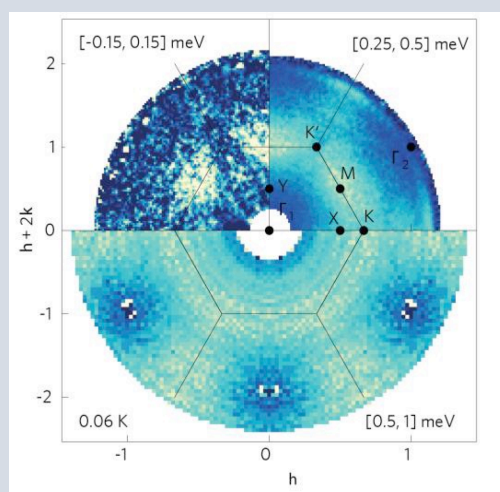


Fig. 1. Scientific discoveries enabled by SNS and HFIR.

Summary of FY 2018 achievements

The neutron science program took advantage of core capabilities and expertise found across ORNL in five key scientific areas: quantum materials, polymers and soft matter, catalysis and interfacial chemistry, materials and engineering, and biological materials and systems. Recent advances in these areas of science that have been enabled using neutron scattering include the following examples:

- Inelastic neutron scattering (INS) was used to elucidate the magnetic excitations in quantum spin liquids.[1] These studies have implications for future solid-state technologies for lossless quantum computing.
- The structure of a cell membrane was measured *in vivo* using small-angle neutron scattering, confirming the membrane's lamellar nature and quantitatively determining the hydrophobic thickness.[2] This research provides direct evidence for the existence of lipid domains in bilayers.
- *In situ* neutron diffraction was used to reveal the structural evolution of a high-entropy alloy as a function of applied stress,[3] contributing to the knowledge required to develop new materials with both high strength and high ductility.
- The unique nature of niobium-based catalysts for the removal of oxygen content from lignins was established by INS,[4] suggesting a promising path for biofuel production.
- Total neutron scattering showed how molecular components have a significant role in determining the properties of hybrid organic perovskite photovoltaic materials.[5]
- *In situ* INS spectroscopy provided the first direct evidence for the presence of both surface and bulk cerium hydride species upon H_2 dissociation over ceria at elevated temperatures which provides new insights into hydrogenations reactions over oxide surfaces.[6]

In these and other areas, the scientific productivity and impact of SNS and HFIR continued to increase (Fig. 2). Users gained access to improved capabilities and identified further improvements required to address emerging science challenges and to ensure they have continued access to the best neutron scattering capabilities. Improvements were completed on HFIR's HB-2C, WAND^2, including the installation of a new data acquisition system, detector, and radial collimator.

HFIR operated seven cycles at 99% availability, with a stabilized fuel inventory. SNS operated at 94% availability against published schedule at 1.4 MW. Both SNS and HFIR had outstanding safety records in FY 2018.

[1] J. Paddison, et al., *Nat. Phys.* **13**, 117 (2017); A. Banerjee, et al., *Science* 356, 1055 (2017).
[2] J. Nickels, et al., *PLoS Biol.* **15(5):** e2002214 (2017).
[3] H. Huang, et al., *Adv. Mater.* **29**, 170678 (2017).
[4] Y. Shao, et al., *Nat. Commun.* **8**, 16104 (2017).
[5] D. Fabini, et al., *J. Am. Chem. Soc.* **139**, 16875 (2017).
[6] Z. Wu, et al., *J. Am. Chem. Soc.* **139**, 9721 (2017).

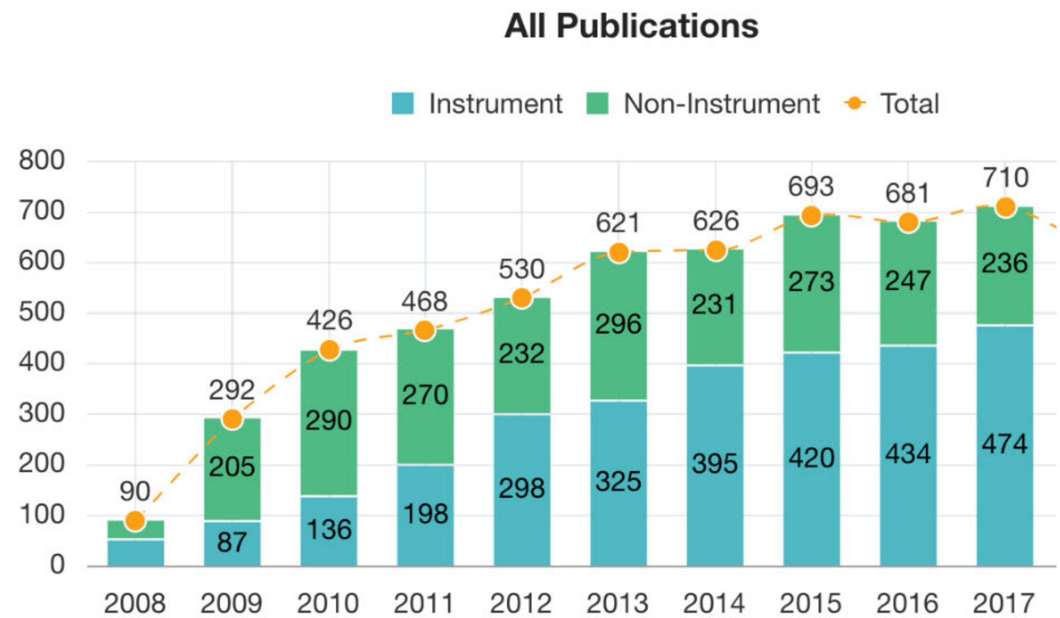


Fig. 2. Publications arising from all HFIR and SNS work in CYs 2008-2017.

During FY 2018, SNS underwent a five-month planned outage for critical activities to maintain or enhance accelerator reliability and power capability, resulting in increased neutron flux. These activities included *in situ* plasma processing of superconducting modules (i.e., internal surface cleaning), installation of the new Inner Reflector Plug (IRP), and installation of the new Radio Frequency Quadrupole (RFQ) structure, which supports routine operation of the accelerator at 1.4 MW. Conversion of the reflector coolant to heavy water provided a 15–20% increase in the neutron flux.

During FY 2018, HFIR set a record for unique users and neutron scattering experiments performed. Five hundred sixty-one unique users performed 588 experiments at HFIR in FY 2018. Six hundred forty-four unique users performed 600 experiments at SNS. The five-month outage at SNS resulted in fewer unique users and experiments in FY 2018 than previous years.

Planned actions for FY 2019

A Strategic Plan for Neutron Science was published in 2014. Our Strategic Plan will be updated this fiscal year and used to help make decisions on prioritizing current improvement projects and proposed new projects to ensure the most effective use of available resources to advance towards our long-term vision and scientific goals. This plan will be updated to reflect recommendations we anticipate from the August 2018 DOE review for FYs 2015–2017 of HFIR and SNS. In addition, input received from various advisory boards, workshops, and the user community will be included.

Improve and optimize neutron scattering capabilities

The Science Productivity Program, which began in 2015, invests operational funds each year to continually improve and optimize neutron scattering capabilities at both SNS and HFIR. This program currently supports about 30 projects, with the longest-duration project scheduled for completion in FY 2023. Completed projects have delivered improved instruments with new scientific capabilities for applications including battery research, time-resolved studies of hierarchical biological systems, and emergent fractional excitations in low-dimensional quantum magnets. Projects scheduled to be completed in FY 2019 (and beyond) will bring additional science capabilities to the user community, including the ability to study field-dependent phase diagrams of materials, magnetic quantum systems, and complex material systems associated with advanced manufacturing. Ten projects are scheduled to proceed in FY 2019.

Develop innovative neutron scattering methods and technologies

We will continue to engage the broader research community through internal and external technical/scientific workshops and advisory committees to assess concepts for new instruments and capabilities to enable world-leading science. As part of this assessment, specific parameters will be considered for several new instrument concepts, including scientific drivers/need, community support, conceptual design concepts, and technical vetting. Construction of one new instrument, VENUS, will begin in FY 2019 and establish an imaging station for SNS. VENUS will be a game-changing platform supporting advanced neutron imaging methods (Bragg-edge, resonance imaging) to fully characterize complex functional materials:

- Real-time simultaneous attenuation-based imaging and microstructure imaging (Bragg-edge) to study materials in extreme environments *in situ* and *operando*
- Elemental (isotopic) imaging using resonances and prompt gammas
- Unprecedented spatial and time resolutions
- Four-dimensional (4-D) imaging of materials

Continued community input will be used to prioritize decisions about which current instruments to improve and which candidate instruments to build across the two existing neutron sources, SNS First Target Station (FTS) and HFIR, as well as for a future STS. This holistic approach ensures optimal placement of instruments across the sources to best match instrument and sources parameters.

We will continue to develop and support joint access mechanisms with other DOE user facilities, such as light sources (including the Advanced Photon Source and National Synchrotron Light Source II) and nanoscience centers (including CNMS). The HFIR and SNS User Meeting will be held June 4-5, 2019, at ORNL.

Sustain and improve neutron production at SNS and HFIR

We plan to deliver seven operating cycles (4000 neutron production hours) ≥ 90% availability against published schedule at HFIR. Preparations will continue for a major outage to replace HFIR's beryllium reflector in 2023. This replacement will extend HFIR's lifetime and its missions in neutron scattering, materials irradiation, and isotope production. The beryllium material has been procured, and fabrication of replacement components, including four beam tubes and specialized tooling and fixtures, began in FY 2018.

Other life extension improvements to ensure safe and reliable operations and an increase in HFIR's uranium oxide fuel inventory will continue in FY 2019. The most important activities are to (1) replace secondary supply lines, (2) rebuild the cold source cryogenic plant and digital control system, (3) replace the reactor control and reactor protection systems, and (4) produce sufficient uranium oxide to sustain fuel fabrication during the Uranium Processing Facility transition at the Y-12 National Security Complex (Y-12).

We plan to deliver 4900 neutron production hours at ≥ 90% availability against published schedule at SNS in FY 2019. SNS will operate at 1.4 MW. At SNS, accelerator improvements are needed to address obsolescence of key systems and sustain operation at current and planned (i.e., higher) power levels. For example, replacement of the remote handling servo-manipulator systems. Accelerator spares will be necessary to maintain reliability and to prepare for higher power operations in the out-years.

Target reliability at SNS will continue to receive the highest priority, with the immediate goal of continuing to achieve predictable and reliable operation at 1.4 MW and a longer-range goal of developing a target to handle 2.0 MW as part of the Proton Power Upgrade (PPU) project. Another critical activity will be the design and start fabrication of the next IRP which we anticipate replacing in 2022.

We will continue to support key partnerships with other national laboratories and international partners in superconducting radio-frequency cryomodules, high-voltage pulsed power, high-power target design, neutron scattering, and sample environment technologies.

The PPU project at SNS will ramp up in FY 2019. This upgrade will double the available proton beam power at the SNS accelerator complex from 1.4 to 2.8 MW. Further, PPU will increase the neutron flux and brightness at the SNS FTS, enabling wholly new capabilities for studying materials and associated chemical and physical processes with neutron scattering. PPU will add new scientific capabilities to the SNS FTS that are urgently needed by the research community to address emerging science challenges. This enhanced flux will allow, for example, *in situ* observation of time-resolved processes, measurements using smaller or less concentrated samples, and new types of experiments under realistic, extreme environmental conditions. Additional benefits include providing broader researcher access to neutron scattering capabilities, increasing the number of experiments possible, and accelerating the pace of scientific discoveries that rely on neutrons to provide unique information about the structures and dynamics of matter.

Following CD-1 approval of the PPU project in FY 2018 and CD-3A approval in early FY 2019, NScD will move toward development of the project baseline for CD-2, procure long-lead equipment to reduce the project schedule and risk, and pursue approval of CD-2 and CD-3. Currently, we anticipate completing the PPU project in 2024.

The PPU project will also provide a necessary platform for a future STS with the highest peak brightness beams of cold neutrons in the world at low-repetition rates. STS will provide a world-leading source of pulsed cold neutrons for examination of soft matter (e.g., polymers, colloids, and biological materials); quantum materials and magnetism; and complex structural materials (e.g., new alloys and 3D-printed composites). STS will provide unprecedented access to mesoscale and complex matter, complementing the existing and future capabilities of FTS, with its high peak brightness beams of thermal neutrons at high-repetition rates, and HFIR, with its continuous beams with high time-averaged flux. This three-source strategy will ensure that U.S. researchers have access to world-leading neutron scattering capabilities to address critical emerging challenges for the foreseeable future. ORNL has received CD-0 approval for the STS project and has made recent progress in addressing remaining technical concerns. We will continue to be prepared to move toward CD-1 approval of the STS project.

Summary

The actions we plan to take in FY 2019 will move us toward achieving our vision to be the world's leading provider of neutron science and technologies, enabling scientific discoveries, and solving scientific challenges that can be best addressed using neutrons.