

## EWALD: An Extended Wide Angle Laue Diffractometer for the Second Target Station

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### ***Abstract***

Revealing the positions of all the atoms in large macromolecules is powerful but only possible with neutron macromolecular crystallography (NMC). Neutrons provide a sensitive probe for the direct detection of protonation states at near-physiological temperatures and clean of artifacts caused by X-rays or electrons. Currently, NMC use is restricted by the requirement for large crystal volumes even at state-of-the-art instruments such as the Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source (SNS). EWALD's design will open the door for new types of experiments, the study of novel systems, and the widescale use of NMC. EWALD is a single crystal diffractometer capable of collecting data from macromolecular crystals orders of magnitude smaller than what is currently feasible. The construction of EWALD at the STS will cause a revolution in NMC by breaking the sample volume limit and opening the door for key discoveries in the biological, biomedical, and bioenergy sciences.

## PIONEER: High Q-resolution Single Crystal Polarized Neutron Diffractometer

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**PIONEER** is a High Q-resolution, Single Crystal, Polarized Neutron Diffractometer for the Second Target Station (STS) aimed at being capable of measuring very small, i.e. X-ray diffraction size, crystals ( $\sim 0.001 \text{ mm}^3$ ), ultra-thin films ( $\sim 10 \text{ nm}$  thicknesses), and weak structural and magnetic transitions. With more than 20 times higher cold neutron brightness than existing instruments, PIONEER will significantly lower the sample-size barrier for single crystal neutron diffraction and enable new science for which neutron diffraction has never previously been thought possible, addressing topics such as the character of the room-temperature superconducting hydride, topological-surface-state-driven magnetic textures, ultra-thin superconducting films, and non-equilibrium states. PIONEER will also take advantage of high flux cold neutrons to strengthen the high Q-resolution for larger scale structures and have polarized neutron capability for analyzing complex magnetism. PIONEER will be a next-generation neutron diffractometer that can enable the characterization of  $0.001\text{-mm}^3$  crystals and stretch the boundaries of neutron scattering science.

## **VERDI: Versatile diffractometer with full polarization analysis capabilities for complex magnetic structure studies in powders and single crystals**

*Abstract:* VERDI will excel at diffraction studies of magnetism in powders and single crystals, allowing routine measurements of milligram-size samples, small-moment compounds, and diffuse signals. The instrument will probe magnetic local and long-range ordering in quantum materials that exhibit emergent properties arising from collective behavior. These insights will help reveal fundamental behavior in quantum magnets that will help drive development and understanding of the next generation of quantum materials with the potential to transform computers and data storage and raise the efficiency of energy storage and transmission. This diffractometer will be equipped with full polarization capabilities and will be optimized for studies under extreme conditions of temperature, pressure and magnetic field. Its unique use of polarized neutrons to isolate the magnetic signature will provide optimal experimental input to state-of-the-art modeling approaches to enable detailed insight into local magnetic ordering to understand the magnetic structure of nano objects, the bond-anisotropic interactions of candidate Kitaev materials, or the interplay of chemical doping and quantum magnetism.

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# BWAVES, a broadband wide-angle velocity selector spectrometer for the SNS Second Target Station

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To probe complex systems, such as biological and soft matter, which are characterized by dynamic processes spanning over an enormously broad time range, neutron spectroscopy must strive to become a broadband technique. BWAVES, a Broadband Wide-Angle VELOCITY Selector spectrometer for the SNS STS, will simultaneously probe dynamic processes spanning 4.5 decades in time, measuring continuous spectra that comprise both vibrational and relaxational excitations, from 0.01 meV to hundreds of meV. The relatively small beam size of 5 mm by 5 mm will enable studies of the samples of only a few microliters in volume, which is critical for measurements of hard-to-synthesize samples and for the use of advanced sample environment equipment. BWAVES is made possible by the first-time utilization of the wide-angle velocity selector to determine a very long wavelength of neutrons detected after scattering by the sample and the full use of the source brightness and low repetition rate.

# CHESS: CHopper spectrometer Examining Small Samples

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## Abstract:

CHESS is a direct geometry neutron spectrometer designed to detect and analyze weak signals intrinsic to small cross-sections (*e.g.* small mass, small magnetic moments or neutron absorbing materials). CHESS will be optimized for enabling unprecedented characterization of spin liquids, quantum magnets, thermoelectric materials, battery materials, liquids and soft matter. The ability to simultaneously measure dynamic processes over a wide energy range for very small samples will make CHESS the spectrometer of choice for first measurements of new materials. The broad dynamic range will be well matched to measurements of relaxation and excitations in soft and biological matter. The 15 Hz repetition rate of STS enables use of multiple incident energies within a single source pulse, greatly extending the information gained in experiments. An essential feature of this instrument will be the capability for polarization analysis to separate nuclear from magnetic scattering or coherent from incoherent scattering processes in hydrogenous materials. This instrument will employ advanced sample environments such as high-pressure cells, dilution refrigerators, high field cryo-magnets and polarization devices, as well as combinations of these, to solve problems at the forefront of materials research. CHESS will be the flagship spectrometer of the Second Target Station (STS), a world-leading instrument in a class of its own, technically feasible to construct and safe to operate.

**Title:** Wide-Angle Neutron Spin Echo, EXPANSE

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**Abstract**

We propose to build a wide-angle spin echo instrument (EXPANSE) at the SNS Second Target Station (STS). This instrument will become the workhorse instrument for scientific problems that involve high-resolution (neV- $\mu$ eV) dynamic processes in a wide range of materials. EXPANSE will incorporate wide angle detector banks that will provide approximately two orders of magnitude  $Q$ -range, and a wavelength band that can provide approximately five orders of magnitude in Fourier times. This instrument will offer unique capabilities that are not available in the currently existing NSE instruments nor in the US, which is to visualize local slow-dynamics in real-space and time, and also to enable time-resolved studies with NSE. The range of science areas in which this instrument will contribute is diverse and will include soft matter, biological materials, ionic liquids, unconventional magnets, quantum materials, and molecules in confinement.

## **Title:** Centaur – A Small- and Wide-Angle Spectrometer for Second Target Station

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### **Abstract**

We propose to build an advanced small- and wide-angle scattering instrument, named Centaur, at the second target station (STS) of ORNL that provides best in class resolution, dynamic range, and unique spectroscopic capabilities. The instrument will maximally leverage the STS source, state-of-the-art neutron optics, and detectors to deliver an unprecedented capability that enables assessment of a wide range of length scales with excellent resolution, measurements on smaller samples, and time-resolved investigations of evolving structures. Beam polarization and a high-resolution chopper will enable detailed structural and dynamical investigations of magnetic materials and quantum materials. The unique characteristics of the new spectrometer make it optimal for time-resolved studies of out-of-equilibrium structures commonly encountered in soft matter and biology when subjected to external perturbations. Moreover, its excellent resolution makes it ideal for low-angle diffraction studies of highly-ordered large-scale structures, such as skyrmions, shear-induced ordering in colloids, and biomembranes.

## M-STAR (Magnetism Second Target Advanced Reflectometer)

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### Abstract

M-STAR is a next generation polarized neutron reflectometer with advanced capabilities. A new focusing guide concept is optimized for samples with small dimensions in the millimeter range. The combination of high brightness and low repetition rate combined with a short instrument length result in significant gain factors in intensity and a wide wavelength bandwidth. A proposed hybrid pulse-skipping chopper will enable experiments at constant geometry at one incident angle resulting in a broad range of wave vector transfer  $Q$  up to  $0.3 \text{ \AA}^{-1}$  for specular, off-specular, and GISANS measurements. The instrument will support an option for magnetic grazing incidence diffraction (GID) to access the out-of-plane magnetic moment and antiferromagnetic structures not available in conventional reflectometry. The proposed concept will enable nano-science and spintronics studies routinely on samples as small as  $2 \text{ mm} \times 2 \text{ mm}$  using versatile experimental conditions of magnetic and/or electric fields, light, and temperature applied in-situ to novel nanosystems. The proposed novel concept in combination with ideally matched STS parameters and unique capabilities will put M-STAR in the world leading position for high resolution polarized reflectometry on small samples.



## **The Quite Intense Kinetics Reflectometer (QIKR)**

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### **Abstract**

QIKR will be a general-purpose, horizontal-sample-surface reflectometer. Exploiting the increased brilliance of the Second Target Station (STS), QIKR will collect specular and off-specular reflectivity data faster than the best existing such machines. Utilizing pulse skipping (7.5 Hz), it will often be possible to collect complete specular reflectivity curves using a single instrument setting, enabling “cinematic” operation, wherein the user turns on the instrument and “films” the sample. Samples in time-dependent environments (e.g. temperature, electrochemical, magnetic, or undergoing chemical alteration) will be observed in real time, in favorable cases with frame rates as fast as 1 Hz. Cinematic data acquisition promises to make time-dependent measurements routine, with time resolution specified during post-experiment data analysis. This capability will be deployed to observe such processes as *in situ* polymer diffusion, battery electrode charge-discharge cycles, magnetic and other hysteresis loops in real time, and membrane protein insertion into lipid layers.

## MENUS - MATERIALS ENGINEERING BY NEUTRON SCATTERING

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### Abstract

MENUS at STS will be a transformational high-flux, versatile, multiscale materials engineering diffraction beamline with unprecedented new capabilities for the study of complex materials and structures. It will support both fundamental and applied materials research in a broad range of fields. MENUS will combine unprecedented long-wavelength neutron flux and unique detector coverage to enable real-time studies of complex structural and functional materials under external stimuli. The incorporated SANS and transmission/imaging capabilities will extend its sensitivity to larger length scales and higher spatial resolution. Multimodal MENUS will provide crystallographic and microstructure data to the materials science and engineering community to understand lattice strain/phase transition/microstructure/texture evolution in three orthogonal directions in complex material systems under combined extreme applied conditions. The capabilities on MENUS will open new scientific opportunities and meet the research needs for science challenges to enable studies a range of phenomena and answer the key questions in material design/exploration, advanced material processing, transformative manufacturing, and material operations of national impacts in our daily life.

## TITAN

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We propose TITAN, a scientific facility to explore materials properties and behaviors under extreme conditions. By exposing, characterizing and synthesizing new states of matter and exploring their potential for applications, the facility will enable transformative progress in the science of quantum materials, engineering and nuclear materials, and in the synthesis of novel exotic materials. TITAN will offer DC magnetic fields in excess of 25 T, pulsed fields in excess of 40 T, on select materials pressure up to 100 GPa for spectroscopy and up to 250 GPa for diffraction, temperatures from 20 mK to 4000 K, and all feasible combinations thereof. Exploiting the record brightness and bandwidth of the STS, TITAN will probe the atomic scale responses to extremes through multimode polarized and unpolarized neutron scattering including high efficiency neutron spectroscopy from 5 meV to 100 meV, high resolution powder and single crystal diffraction, and SANS. TITAN will enable synchronization with pulsed sample environments to explore the time dependent response to perturbations and thermalization on the sub ms time scale. Focusing neutron optics will maximize flux on accurately positioned samples with dimensions from 100  $\mu\text{m}$  to 40 mm while radial collimation and optimized shielding and detection strategies minimize backgrounds. The TITAN facility will be configured and persistently engaged in R&D to define the frontier of research in materials under extreme conditions with neutrons.

# CUPI<sup>2</sup>D: Complex, Unique and Powerful Imaging Instrument for Dynamics



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## ABSTRACT

This proposal presents the scientific justification, science-driven performance expectations and a brief overview of the main components for CUPID<sup>2</sup>, the proposed transformational time-of-flight imaging instrument at the Second Target Station. The beamline is designed for a broad range of applications. CUPID<sup>2</sup> will have a transformational impact on scientific areas such as energy storage & conversion (batteries, fuel cells to transform energy and transportation fields), materials engineering (additive manufacturing, advanced superalloys), nuclear materials (novel fuel cladding and moderators), cementitious materials, biology and ecosystems (in situ plant fluid/nutrient dynamics) and medical/dental applications (3D printed adaptive implants) and other fields.

The innovation of this instrument lies in the utilization of a high flux of cold neutrons for performing **real time in situ** neutron grating interferometry and with a wavelength resolution of  $\Delta\lambda/\lambda \approx 0.02\%$  for Bragg edge imaging capabilities, simultaneously when required, across a broad range of length and time scales.