Quantum materials

3. A neutron source to unlock quantum materials for the post silicon era

Quantum materials are critical for the future of science and technology, offering the potential to revolutionize key technologies including classical and quantum computing, sensing, energy harvesting, and energy storage systems. Their unique properties, emerging from the complex interactions between charge, orbital, spin, and lattice degrees of freedom, drive breakthroughs in these fields. Over the past few decades, quantum materials have led to important advances in computation and energy efficiency. Notable examples include giant magnetoresistance (GMR) for magnetic storage (Nobel Prize in Physics 2007) and blue-light LEDs for efficient lighting (Nobel Prize in Physics 2014). However, the surging demand for computation requires accelerated discovery of next-generation quantum materials. As recognized in the CHIPS and Science Act, quantum materials will be key to technological leadership and global competitiveness in the post-silicon era.

A next-generation second target station for the spallation neutron source will image the complex interplay between spin, lattice, and orbital degrees of freedom to accelerate understanding and applications of the associated collective phenomena. In the following we describe four priority research directions and the pivotal role that the STS will play at the fertile interface between fundamental and applied science of quantum materials.

3.1. Discover quantum materials that approach fundamental limits for information and energy technologies

Contemporary society increasingly depends on the pervasive availability of large-scale electronic data and its real-time processing (Hilbert 2011) . This is epitomized by the explosive growth of artificial intelligence (AI), machine learning (ML), and neural network applications that promise to transform our economy and society including how scientific research is conducted. The transformation is however, doubling our computational needs (Electricity 2024) every 4 months (Mehonic 2022). This is unsustainable and requires a transformation in computational energy efficiency. Extending traditional CMOS-based technologies to meet these demands confronts fundamental limits on speed, density, and energy efficiency (Knowles 2021, Electricity 2024) so that alternative approaches must be developed (Marković 2020).   The unique properties of quantum materials have great potential as the post silicon platform for fast, dense, energy efficient information technologies (Hoffmann 2022).

A vast space of quantum materials is to be harnessed for applications ranging from dissipationless interconnects, topologically quantum computing, spin-encoded IT, to energy scavenging. While our ability to predict materials properties from atomic scale structural information improved and enabled the Materials Genome Initiative, the next quantum revolution will require quantum capable materials property predictions.

While classical computations can handle millions of atoms and electrons, quantum computations stall at dozens of atoms and electrons due to the exponentially scaled complexity of interacting quantum particles. AI-driven methods that combine high-throughput semi-classical methods with small scale quantum computations offer a path forward. This hybrid method involves training neural networks with extensive experimental datasets that can be directly compared to theoretical/AI predictions.

A quantum-capable materials discovery program may guide a network of sample synthesis and experimental teams to discover materials where quantum effects drive functionality. It will provide a new level of accuracy in the design of technological devices that approach fundamental limits of energy efficiency, density, and speed. Static and dynamic magnetism being the quintessential quantum materials property, neutron scattering will be indispensable to the quantum materials revolution as the STS brings data rates to the necessary scale.

Interfaces between quantum materials provide rich opportunities for new electronic functionality. Topological Insulators (TI) and Superconductors (SC) are profoundly modified by time-reversal symmetry breaking; a gap opens in the Dirac surface states of TI, while triplet pairing and/or Majorana bound states may form in a SC (Qi 2011) . magnetically ordered ferro- and antiferro-magnetic thin films can induce these effects through interface mediated exchange interactions. Materials with strong spin-orbit interactions in turn can induce out-of-plane magnetic anisotropy in magnetic thin films, which is essential for a range of IT applications. In all these cases, polarized neutron reflectometry (PNR) is critical to image the vector magnetization depth profile in such thin film heterostructures. The brightness of the STS will enable depth-resolved characterization of magnetization statics and dynamics in samples near the application device format.

3.1.1. Essential Connections to STS

The transformative increase in brightness of cold neutrons at the STS combined with full spectrum instrumentation will increase data rates by 2-3 orders of magnitude, which can be leveraged by AI-guided decision-making and information extraction (Chen 2021). Quantum materials discovery will capitalize on this through accelerated, AI-informed materials discovery workflows, detailed investigations of materials functionality under external stimuli and extreme conditions, and through measurements of spatially confined and driven excitations in quantum materials. Examples of STS impacts on quantum materials discovery are below.

Accelerated discovery: Discovering new quantum materials follows an iterative cycle of prediction, synthesis and measurements. We envisage that prediction of materials with targeted properties will increase dramatically in an AI-driven future combined with rapid advancements in quantum materials modeling through classical and quantum computing. However, the discovery environment requires vast quantities of high-quality data on a representative variety of samples.

The nature of the neutron scattering cross section confers unique standing to supply the ground truth to neural networks and to benchmark theoretical advances. The enhanced brightness of the STS is essential to bring data acquisition rates to parity with the synthesis and modeling components of quantum materials development.

Novel Functionality: The unique responses of quantum materials to stimuli including electric fields, magnetic fields, or light, are the basis for their applications. AI driven methods will improve our ability to predict desired functionalities. Verifying these predictions and more generally understanding how functionalities emerge in quantum systems requires detailed investigation of the evolution of crystal and magnetic structures, textures, and fundamental excitations under a variety of experimental conditions. By dramatically reducing the required sample volume, intense focused STS beams will enable dense, parametric studies of families of materials and of materials pushed to extreme thermodynamic conditions of temperature, pressure, and magnetic field.

Combining neutron scattering and high magnetic fields enables unique insights into mechanisms and functionalities, which is why about 20% of quantum materials neutron experiments are performed in a magnetic field. While higher-field neutron scattering should yield breakthroughs in quantum materials science: there has been no progress in the maximum field available for thirty years (HMF 2024). To amplify scientific impact, the world leading neutron source should be combined with steady fields in the 20-30 tesla range and pulsed fields in the 40-60 tesla range.

Pressure changes interatomic distances and alters exchange interactions to expose novel quantum states of matter. The intense focused neutron beams at the STS will enable inelastic scattering to probe spin dynamics under pressures up to 10 GPa and detailed neutron diffraction studies up to 100 GPa. Such capabilities could be transformative in efforts to understand and expand a new family of rare earth hydrides with near room temperature superconductivity.

3.1.2. Transformative Pilot Science Cases

Quantum magnetism: Transformative applications are built on a strong understanding of the underlying physics. Though much more common than ferromagnets, we are only now discovering the power and energy efficiency of antiferromagnets in spintronics. Spin wave propagation may be used to transfer classical and quantum information (Leenders 2024).

Antiferromagnetic spin dynamics is possible at the THz frequency scale (Jungwirth 2016, Zhang 2024), thus addressing grand technological challenges. Understanding and controlling spin dynamics at the nano-meter scale in quantum magnetic materials constitutes an important scientific and technological challenge where the brightness of the STS can have transformative impacts. Also, emergent quantum materials of fundamental importance to elucidate quantum entanglement must often be studied in small high quality samples that only come into view with the STS.

Kitaev quantum magnetism: A 35-T magnetic field can fully magnetize the Kitaev material α-$RuCl_3$. Combining a modern high DC field magnet system with neutron spectroscopy at the STS would allow unambiguous determination of the Heisenberg-Kitaev spin Hamiltonian for α-$RuCl_3$ and other putative Kitaev materials. This would elevate efforts to understand and exploit the Kitaev spin liquid for quantum computing.

Electronic interface dynamics: Quantum materials functionality is often associated with electronic properties at interfaces. Topological quantum materials for example can feature symmetry protected edge states. Neutron reflectometry is a well established method to determine the structure of interfaces through the surface sensitivity of evanescent neutrons at grazing incidence. Orders of magnitude more flux at the SNS will enable inelastic neutron scattering for thin films and interfaces. This opens the door to probing topologically protected edge states, spin waves, and phonons at the interface of multiple quantum materials. The broad dynamic range of neutron scattering and the well-defined nature of neutron-matter interactions uniquely complements other surface sensitive spectroscopies.

Neuromorphic computing: Interactions between electrons in quantum materials produce strong electric, magnetic, and mechanical responses to external stimuli that are impossible in silicon . Strongly non-linear responses have been proposed to emulate the integrate-and-fire dynamics of neurons (Rao 2022). Non-local phenomena in quantum materials may be used for distributed information processing as in the natural brain. Fast dynamics might be exploited for dense temporal synapses in artificial neural networks. Quantum materials thus hold the potential to revolutionize information storage and processing which are key to global competitiveness and to a thriving, secure, and prosperous society (Marković 2020). The STS will provide the capability to image THz dynamics in quantum materials and advance their technological applications.

3.2. Advance fundamental understanding of quantum coherent and incoherent dynamics in materials platforms

Quantum materials can realize unique quantum fluctuating states of matter that are linked to fundamental particle physics through quantum field theories and provide unfamiliar materials functionalities to fuel technological innovation. However, our ability to characterize, understand, and control quantum materials is limited by the power of the experimental techniques we develop to probe their properties.

The STS will dramatically expand the dynamic range and sensitivity of neutron scattering to image quantum materials over the broad range of length and time scales needed for progress. Novel types of quasi-particles such as spinons, majorana fermions, visons, and magnetic monopoles will become accessible by neutron scattering from minute quantities of high quality material under extreme thermodynamic conditions, confined in nano-structures, and driven beyond thermal equilibrium.

Experimental access to quantum coherence and decoherence will be possible to challenge and advance our understanding of the transition between the quantum and classical domains and stimulate the development of new materials platforms for quantum information technologies.

Examples of strongly fluctuating quantum states of matter include spin fluctuation mediated superconductivity in copper oxides, iron pnictides and heavy fermions and quantum spin liquids in frustrated and low dimensional magnetic materials. In such materials, the physics often lies in the exotic quasi-particles they support. Examples include Bogoliubov quasiparticles, spinons, anyons, majorana fermions, and magnetic monopoles. These expose the mechanism behind magnetically mediated superconductivity or form the basis for applications ranging from information and heat transfer to quantum computing. These frontier areas will be transformed by the STS, because neutrons are the principal tool to detect quasi-particles.

The enhanced dynamic spectral range and sensitivity of inelastic neutron scattering and the ability to distinguish distinct components of scattering through polarization analysis make it possible to address foundational aspects of quantum theory: In particular our understanding of the transition from the quantum to the classical domain is tenuous. There are deep scientific and philosophical questions at stake but also a practical dimension as the quest to control decoherence in quantum computers has brought renewed attention. The superior resolving power of the STS will bring the quantum classical crossover into view in quantum materials. Such experiments will also advance understanding of charge, spin, and heat transport in quantum materials.

As the capabilities of quantum computers grow a curious challenge can be anticipated. How can we check their accuracy when their computational power eclipses any classical supercomputer? The direct relationship between models of quantum materials and the neutron scattering cross section means that accurate measurements of the scattering cross section for well defined materials can provide solutions to problems that lie beyond the capabilities of supercomputers so that such experiments become a valuable component of benchmarking new quantum computing systems.

3.2.1. Essential Connections to STS

The STS offers a range of unique capabilities to address grand scientific challenges in quantum materials science.

Resolution: The enhanced source brightness and novel instrumentation concepts will push cold neutron spectroscopy at the STS into new regimes of resolution and sensitivity. In the quest for a quantum spin liquid this provides spectroscopic access to the cross-over between quantum spin liquid physics and lower energy regimes where materials specific defects or weak interactions lead to decoherence, spin freezing, or magnetic ordering. The STS will accelerate the quantum materials optimization process.

Polarization: While fully spin polarized instrumentation neutron scattering is in principle possible now, the enhanced source brightness and novel spin polarized detection systems make such experiment feasible on a wider range of interesting materials.

Measurement of Higher-Order Correlation Functions: The coherence provided by STS enables the measurement of higher-order correlation functions. This capability brings neutron scattering closer to quantum information science, adding momentum, energy, and spin resolution, to related methods in quantum optics.

Linewidth Analysis for Quasiparticle Lifetimes: Unlike traditional scattering measurements, which focus on determining resonance energies, STS allows for detailed lineshape analysis to probe quasiparticle lifetimes and decay channels.

Beyond thermal equilibrium: Building on its brightness and time structure, the STS will be able to probe quantum materials driven beyond thermal equilibrium and provide a unique view of collective relaxation phenomena and thermalization processes, which are of great fundamental and practical importance.

3.2.2. Transformative Pilot Science Cases

Gapless spin liquid: Magnetic materials frequently develop conventional types of long-ranged order, such as ferromagnetism or antiferromagnetism. Spin liquids have more complicated kinds of order, with new emergent excitations, and new materials such as NaYbSe2 are exciting possibilities that seem to lie beyond conventional order. Spin liquids that have gapless excitation are beyond the established theory of topological order, while gapped spin liquids could also appear as gapless due to the small gap size of either intrinsic nature or rendered by materials defects. Nonetheless, measuring Q-dependent spin correlation function in the ultra-low energy regime is essential to determine the nature of such materials.

Decoherence of quantum states: An area of great recent progress is the use of solids to create states with long-lived quantum coherence, as in diamond color centers or superconducting qubits. Even biological systems such as chlorophyll may achieve an unexpected degree of environmental isolation and high coherence. STS offers the potential to study decoherence processes in solids at low temperature by covering the time scale from initial interactions between an electronic or spin state and its environment, to the emergence of classical dynamics. The STS will uniquely enable such work in complex interacting materials.

Extracting entanglement witnesses in quantum magnets: A model independent determination of solid state quantum entanglement is a persistent challenge. An emerging approach is to extract entanglement witnesses from the two-point correlation function measured by inelastic neutron scattering. Full polarization analysis brings out the full potential of this approach. This capability will be uniquely enabled by STS for a versatile quantitative gauge of "quantumness" in materials.

Higher-order neutron scattering for four-spin correlators $\langle SSSS \rangle$: Higher-order correlations are essential to explore many-body excitations and entanglement patterns in materials but at the moment we have no experimental probe. With increased neutron coherence across mm-scale, it becomes feasible to exploit higher-order correlation functions through noise spectroscopy as in x-ray photon correlation spectroscopy (XPCS). The inelastic magnetic neutron scattering analogue of such experiments could open an important new window on quantum materials.

3.3. Unveil multi-component electronic orders and excitations in quantum materials

Intertwined electronic orders are central to quantum materials science. Understanding this rich physics requires breakthroughs in experiment and theory. With sensitivity to magnetism and to charge order through lattice displacements, neutrons are an indispensable probe of intertwined structure and dynamics so that a breakthrough on the experimental side can be foreseen from the enhanced brightness of the STS.

Intertwined electronic orders can produce complex phase diagrams with novel types of superconductivity such as pair density waves, nematic superconductors, and charge 4e (or 6e) condensates. Superconductivity is also found intertwined with novel magnetic and topological phases of matter. These phases typically have critical temperatures of comparable magnitude and arise in strongly correlated materials.

While some of these states were first discovered in copper-oxides, evidence for intertwined spin, charge, and superconductivity have recently been reported in the kagome lattice compounds CsV_3Sb_5 and Mn3Sn, the heavy fermion superconductor UTe_2, and in iron based superconductors such as FeSe. Parametric studies of intertwined orders and excitations versus stoichiometry, magnetic fields, pressure, strain and combinations thereof are needed to understand and control this rich quantum materials phase space. Focused high intensity STS beams will enable comprehensive mapping of intertwined orders throughout their multi-dimensional phase diagrams to expose qualitatively new phases and understand the underlying fundamental physics.

3.3.1. Essential Connections to STS

With unrivaled luminosity at long wavelengths, the STS will detect magnetic excitations at lower energies than previously possible and magnetic diffraction from thin films. An ultra-high-field magnet system for neutron scattering beyond 20 T would provide a world-unique capability to tune and probe materials for scientific breakthroughs at the core of quantum materials science.

Measurement of hierarchical excitations can expose the interplay between coupled degrees of freedom. Based on efficient moderators, repetition rate multiplication, and employing the latest advances in computing and analysis, STS spectrometers will offer greatly enhanced data rates and access to the variety of sample environments needed to map intertwined states of matter.

3.3.2 Transformative Pilot Science Cases

The higher flux in focused beams will enable the search for and characterization of intertwined orders in currently inaccessible materials, and investigation of the interplay between quenched disorder and collective order parameters.

Samples with intertwined order are often too small for current instrumentation. For example, superconductivity above 20 K was recently detected in a family of nickel oxides that can only be grown as epitaxial thin films. The parent compound, $LaNiO_2$, should exhibit antiferromagnetic order but the thin film sample volume is insufficient for current neutron instruments and resonant inelastic x-ray scattering (at the Ni L_3 edge) is cannot access the antiferromagnetic wave vector and electron diffraction is insensitive to antiferromagnetism. The intense focused beams of the STS would allow a direct measurement of the magnetic order and the associated magnetic form factor, uniquely delivering critical information to understand magnetically driven superconductivity in transition metal oxides. When Sr is partially substituted for La, the resulting charge carriers can intertwine with the magnetism. Again, the STS instrumentation is needed to image the resulting orders.

Several other nickel-oxide compounds have been shown to become superconducting under pressure; one example is $La_3Ni_2O_7$. The spin and charge correlations in this system under pressure need to be investigated to elucidate the underlying physics, but the sample volume compatible with a pressure cell is too small for current neutron diffraction measurements and much too small for inelastic studies. Here again intense focused beams that can be provided only at the STS offer opportunities to make contact with the relevant order parameter despite the reduced sample volume.

3.4. Harness coupling between transport and mesoscopic structures and dynamics in driven quantum materials and devices

Driven beyond equilibrium, materials can transcend chemical constraints and exhibit unique emergent physics. Under the exquisite control of periodic perturbations. It may be possible to get closer to idealized model properties than through materials chemistry alone. Consider for example the exactly solvable Kitaev model, which supports Majorana quasiparticles relevant for topologically protected quantum computing. So far, however, actual honeycomb materials, however, have non-Kitaev interactions that produce ordered phases without Majoranas. With pulsed or time periodic drives, it may be possible to drive such materials into desired regimes.

Another rich arena for novel electronic functionality are planar interfaces between distinct quantum materials. Adding a material with strong spin orbit interaction to a ferromagnet has for example been shown to produce technologically important out-of-plane (OOP) magnetic anisotropy. Adding a magnet to a topological insulator can open a gap in Dirac surface states and produce a quantized Hall response, while Majorana bound states may be formed at engineered interfaces between magnetism and superconductivity.

3.4.1. Essential Connections to STS

The enhanced brightness of the STS will bring sub-meV energy resolution, momentum resolution, and the unique contrast and polarization selectivity of neutron scattering to explore exposed and buried interfaces of driven and nano-structured quantum materials over the full range of temperature and fields. No other surface sensitive experimental technique can match these characteristics.

It is the low repetition rate and world leading peak brightness of the STS that enables transformative neutron reflectometry. Polarized neutron reflectometry (PNR) and grazing incidence neutron diffraction can provide a complete picture of the magnetization depth profile in driven magnetic thin films. The instrument would access a broad Q range for a single incident angle so measurements can be performed in a fixed scattering geometry. Advanced focusing optics will provide performance gains of 2-3 orders of magnitude relative to current instrumentation and enable wide Q measurements on surfaces down to 1 mm2.

The high peak flux of the STS and optimized beam delivery systems will make neutron spectroscopy a viable method for nano-structured samples. Not only will it be possible to probe magnetic excitations at buried interfaces and confined in thin film structures but it may be possible to spectroscopically resolve fast magnetic dynamics in driven thin film devices. While the ultrafast THz dynamics of antiferromagnetic spintronics is too fast to characterize with conventional electronics, this is the frequency range where inelastic neutron scattering. Inelastic neutron scattering furthermore adds atomic scale spatial (Q) resolution. The ability to image spin dynamics in operating magnetic thin film devices will accelerate design and development of a new generation of spintronic memory and logic devices.

3.4.2. Transformative Pilot Science Cases

Antiferromagnetic spintronics has tremendous potential to increase the speed, density, and energy efficiency of electronic information storage systems. Developing and optimizing materials and structures for such applications requires imaging antiferromagnetic spin structure in the driven device. Neutrons provide sensitivity to magnetism and spectroscopic access to THz dynamics. The brightness of long wavelength neutrons at the STS will allow imaging of a non-volatile magnetic memory as it is switched. A coherently rotating spin structure with angular frequency ω, would results in a magnetic Bragg peak at energy transfer $\hbar\omega$ with a width that reflects the temporal and spatial coherence of the spin dynamics.

Neutron scattering at the STS may become an essential tool to probe static and even dynamic properties of an artificial Kitaev spin liquid induced by circularly polarized optical pumping.

3.5. Summary and Outlook

Materials with strongly interacting electrons exhibit a rich variety of collective properties driven by quantum mechanics. Understanding and controlling these novel states of matter is a great fundamental scientific challenge with exciting practical ramifications. This is because the physical properties of quantum materials have the potential to revolutionize major technological systems including.

The world leading brightness and dynamic range of the second target station (STS) will revolutionize our ability to image quantum materials for discovery and to advance our quantitative understanding of their useful physical properties. STS experiments will (1) accelerate the discovery of quantum materials for energy and information technologies, (2) advance fundamental understanding of coherent and incoherent dynamics in quantum materials, (3) Unveil multi-component electronic orders in quantum materials, and (4) allow us to probe structure and dynamics of driven quantum materials and devices. The world-leading next generation capabilities of the STS will be key to unlocking quantum materials for a post silicon technological era.

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