3.4 Chemistry and Environmental Science: Addressing Global Sustainability

Addressing the intertwined challenges of building a climate-resilient nation and resource sustainability is vital for the future of humanity and the American economy and is a critical focus of U.S. federal initiatives [1]. Achieving climate preparedness while strengthening US manufacturing and energy independence is imperative. Recent studies outline viable pathways and priority areas to reduce emissions [2]: diversifying energy systems away from fossil fuels, decarbonizing and improving industrial processes, and advancing new chemical feedstock sources through carbon capture, utilization, and storage (CCUS) technologies.

However, these actions alone are not enough to address the broader resource crises society faces. These include the need to increase the circularity of material systems—recovering and reusing resources—and improving the sustainability and economic viability of food, water, and energy systems. A key challenge is mitigating pollutants in waterways, such as perfluoroalkyl substances (PFAS, or “forever chemicals”), agricultural runoff containing phosphorus and nitrogen, nanoplastics, pharmaceuticals, and other unregulated contaminants. Additionally, byproducts from resource-intensive industries, such as mining tailings and inefficiencies in chemical separations, demand innovative approaches for reduction and remediation.

To confront these challenges, we must adopt a systems-level, cradle-to-grave perspective on sustainability. This spans molecular design through macro-scale applications, encompassing renewable energy systems (e.g., photovoltaics, batteries, and capacitors), sustainable agriculture (soil health, seed optimization, fertilizer use, and water conservation), and the energy-efficient design of chemical processes. More broadly, achieving sustainability in manufacturing requires transformative innovation in understanding and controlling the dynamic nature of materials.

Traditionally, materials/chemistry research has emphasized static "structure-function relationships" in materials. However, advancing sustainability demands a reimagining of this paradigm to incorporate dynamic and non-equilibrium properties, such as interfacial interactions, disorder, defects, metastable states, and out-of-equilibrium behaviors. By observing and manipulating these “structure-dynamics-function” relationships, we can unlock new avenues for innovation in materials science and environmental chemistry.

Compounding these efforts is the emergence of artificial intelligence (AI) and machine learning (ML) as transformative tools for scientific discovery. Integrating these technologies with a next-generation neutron source—providing unprecedented increases in cold neutron brightness and effective count rates—enables researchers to study dynamic processes across relevant material compositions, length and time scales. This capability will drive breakthroughs in understanding and optimizing materials for sustainable applications, catalyzing progress across energy, manufacturing, and environmental systems.

3.1.1 Resilient Energy Economy

Grand Challenge. Climate change, driven by anthropogenic CO_2 and other greenhouse gas emissions, poses a grave threat to humanity. It increases the risk of extreme weather events, jeopardizes critical infrastructure, and endangers the global population's ability to ensure food security and access to clean water. This challenge represents an urgent and profound grand challenge for the U.S. and the world at large.

In the U.S., energy-intensive sectors such as transportation, industry, commerce, and housing remain heavily reliant on fossil fuel combustion (Figure 1). Decarbonizing these energy streams and breaking our dependence on fossil fuels and contributing to US energy independence.

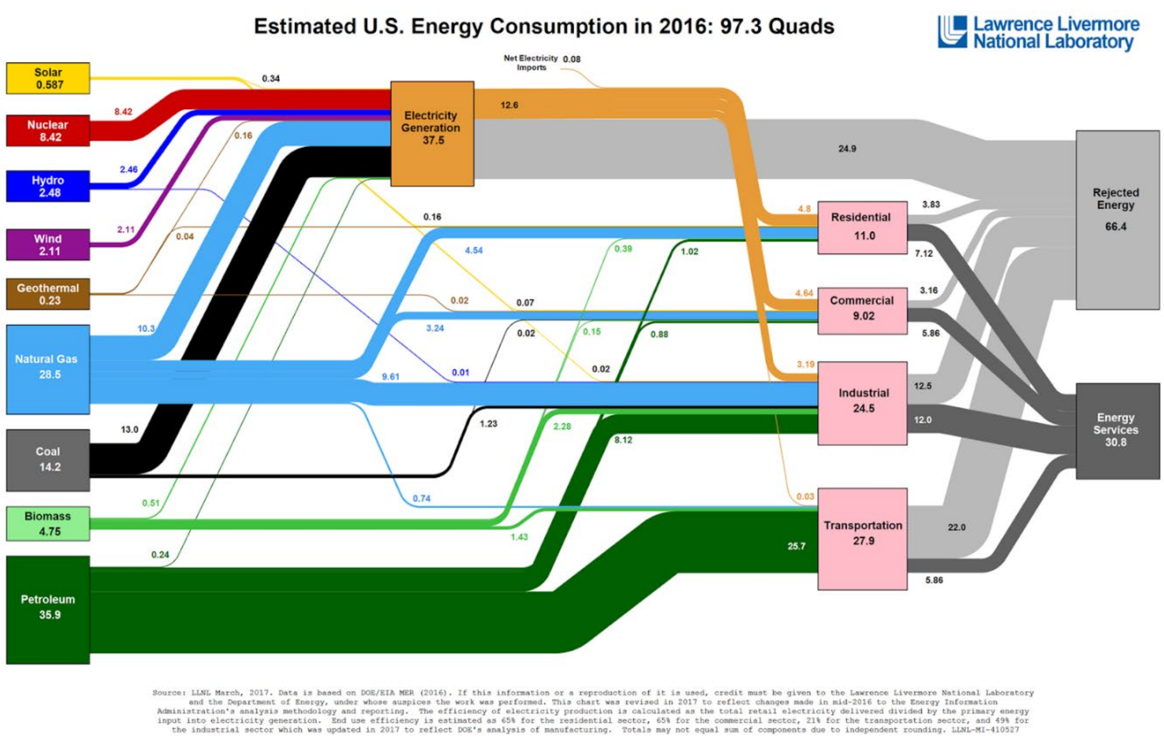

Figure 1. Production and distribution of energy sources into different sectors in the US in 2016. 1 Quad is equivalent to 1 quadrillion BTUs. Figure from Lawrence Livermore National Laboratory.

3.1.1.1 Scientific and Technological Impact

The U.S. scientific and engineering communities are uniquely positioned to address this challenge by pioneering innovative solutions to decarbonize energy systems. This includes:

- Developing efficient photovoltaics for solar energy conversion.
- Advancing hydrogen-based energy systems.
- Improving nuclear energy technologies.
- Harnessing waste heat for energy recovery.
- Innovating new materials for energy storage and conversion.

A deeper understanding of complex materials systems, particularly the chemistry at their interfaces, is critical to these efforts. Insights into the behavior of electrons, protons, ions, and molecules at these interfaces will enable the development of next-generation materials that can drive decarbonization and tackle the grand challenge of climate change.

Photovoltaics (PV)

The most common material used in commercial PV panels is still silicon; however, ongoing advancements in materials science are leading to the development of more efficient and cost-effective solar cells. Thin-film, organic, and hybrid-perovskite materials are all being developed to compete with traditional technologies. Neutron scattering has already contributed to understanding the operation principles of the latter organic-containing materials, particularly the dynamic properties of the cations in the hybrid-perovskite systems.

Hydrogen generation, transport, and storage

- **Generation:** Hydrogen can be produced via steam methane reforming (coupled with CO_2 capture). Another option is the electrolysis of water which is currently two to three times more expensive than producing hydrogen from natural gas [3]. Emerging technologies, such as thermochemical and photoelectrochemical water splitting, require further research into robust materials that can endure extreme environments and improve efficiency.
- **Transport and Storage:** Hydrogen distribution via pipelines, high-pressure trailers, or cryogenic liquefaction faces challenges such as material embrittlement, cryogenic complexity, and infrastructure costs. Alternative solutions, such as hydrogen carriers (e.g., metal hydrides, ammonia), show promise but require advancements in scalability, storage capacity, and safety.

Nuclear energy

- Small Modular Reactors (SMRs): These reactors are safer and more efficient but operate under extreme conditions, requiring advanced materials to resist corrosion and radiation damage.

- Molten Salt Reactors (MSRs): While highly efficient, MSRs require materials resistant to corrosive salts and high temperatures.
- Fusion Reactors: Plasma-facing materials must withstand extreme heat, neutron flux, and particle bombardment without degradation, presenting a critical area for material innovation.

Materials for waste heat capture and conversion
Industrial processes generate significant waste heat, representing an opportunity to enhance energy efficiency. Technologies such as thermoelectrics, phase change materials (e.g., barocalorics), and refrigerants can capture and convert waste heat into usable energy. These materials, particularly their dynamic properties, are ideal candidates for high-brilliance, cold neutron investigations.

Batteries and storage
Transitioning to a low-carbon economy requires robust energy storage systems to balance intermittent renewable energy sources. While lithium-ion batteries dominate, novel solutions using abundant materials like sodium or iron offer more sustainable options. Solid-state designs and advanced energy storage technologies (e.g., supercapacitors, thermoelectrics) demand tailored material structures, which can be explored with neutron scattering to optimize performance.

3.1.1.2 Relevance to STS

The STS provides transformative capabilities to probe the structure and dynamics of materials central to a low-carbon energy future. With next-generation cold neutron sources, STS enables:

- In situ and operando studies: Observing interfacial phenomena and chemical transformations in real time, previously inaccessible due to limited neutron flux.
- High-temperature corrosive environments: Investigating structural and dynamic properties in MSR salts.
- Hydrogen diffusion: Probing storage material behaviors and optimizing energy efficiency and kinetics.
- Photovoltaics: Exploring molecular movements at buried interfaces and catalyst surfaces.
- These capabilities will provide unparalleled insights into materials at nanoscale and macroscale levels, driving innovation in renewable energy and storage technologies.

Accelerated Materials Development.
Achieving breakthroughs in energy systems hinges on the rapid development of advanced materials. Integrating experimental insights from neutron scattering with

first-principles simulations and AI tools will accelerate the discovery of novel materials.

The Materials Genome Initiative (https://www.mgi.gov/) approach emphasizes feedback loops between modeling, synthesis, and characterization, yet bottlenecks persist in the latter stages. STS will address this asymmetry by enabling faster, more comprehensive materials characterization, fueling energy-efficient innovations that outpace the current state of the art. By bridging the gap between experiment and theory, STS will empower scientists to unlock revolutionary materials and processes, paving the way to a sustainable, low-carbon energy economy.

3.1.2 Sustainable Chemistry and Industry

Grand Challenge. Key resource optimization options such as materials efficiency, energy efficiency, circular material flows, and emerging primary processes are needed to maximize the use of precious resources and to reduce CO_2 emissions from the industrial sector [4]. These efforts are essential to meeting climate targets while maintaining economic growth and societal well-being.

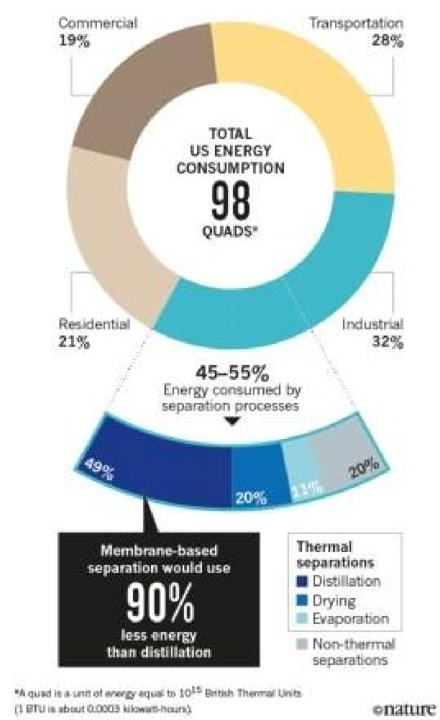

Figure 2. Figure from reference [5] based on Oak Ridge National Laboratory data. *Materials for Separation Technologies: Energy and Emission Reduction Opportunities* (2005).

3.1.2.1 Scientific and Technological Impact

Chemical separations

Chemical separations account for about half of US industrial energy use and 10-15 % of the nation's total energy consumption [5]. These separations frequently demand high pressures and low temperatures for industrial efficiency and developing alternatives that don't use heat could make the majority of these separations 10 times more energy efficient [Figure 2]. Advances in material science, particularly in developing new porous materials, present the potential to enable these separations to occur under ambient conditions, thereby improving energy efficiency and environmental sustainability.

These materials are also key in CO_2 capture technologies, including point-source capture and direct air capture (DAC). High-flux neutron scattering at the STS can play a pivotal role in studying these porous materials under real-world operating conditions. By probing structure-dynamics-function relationships across multiple time and length scales, researchers can optimize these systems for energy efficiency and scalability.

Carbon capture, conversion, utilization and storage

Efforts to rebalance the global carbon cycle require capturing existing CO_2 and converting or storing it to mitigate its atmospheric presence. STS will provide critical insights into the development of advanced CCUS technologies, including:

- Carbon Capture: Studying adsorbents such as amine-based materials, metal-organic frameworks (MOFs), and ionic liquids to optimize efficiency, selectivity, and durability. Neutron scattering uniquely probes hierarchical structures and molecular dynamics over relevant timescales, revealing the mechanisms behind effective carbon capture.
- Carbon Conversion: Developing materials and catalysts for converting CO_2 into value-added products (e.g., fuels, chemicals) through thermal, plasma, or catalytic reactions. STS can address the lack of understanding surrounding interfacial interactions and reaction kinetics, which are critical for improving conversion efficiency.
- Carbon Storage: Ensuring the security of CO_2 storage in geological formations or its transformation into stable mineral forms. Neutron imaging and tomography at STS can provide real-time insights into the structural stability and interactions of CO_2 with porous rock formations.

Sustainable manufacturing

A 2023 report found a chemical accident occurs in the US on average every 1.2 days [7], which exposes US citizens and the environment to dangerous toxins. Transforming chemical manufacturing to be less wasteful and use more environmentally friendly materials and processes is possible, with benefits for industry and consumers. Aligning the new, unprecedented opportunities offered by STS with green chemistry research will be a critical component of the evolution of sustainable manufacturing.

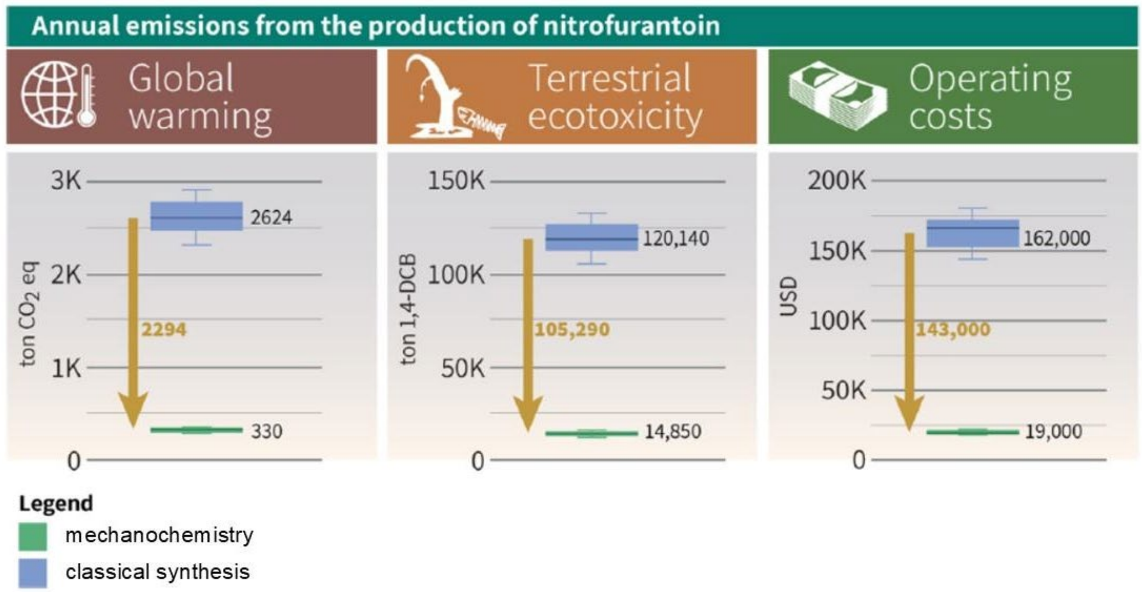

Figure 3. Illustration of improvements in manufacture of a model pharmaceutical by switching from traditional manufacture to mechanochemistry. (adapted from: https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.1c06434)

The global pharmaceutical industry creates 15M tons of waste, with a disposal cost of approximately $30B, and solvents account for approximately 60% of this waste [9]. Reducing solvent use by only a third would reduce waste production by 3M tons globally, with savings of $6B annually. To enable this change, pharmaceutical industries are considering using mechanochemistry to mitigate or eliminate solvents [see impact example in Figure 3], which IUPAC endorses as a top-ten transformative technology of the future [10]. Developing neutron techniques for structural characterization and reaction monitoring is essential for optimizing mechanochemical processes and understanding the underlying mechanisms, which could revolutionize the energy efficiency and environmental footprint of various industries including pharmaceuticals, agrochemicals, fine chemicals and catalysts, polymers, and metal/mineral processing. Neutron methods at the STS would allow for unique and unprecedented insights into the positions of light atoms at the molecular level and *in situ/operando* observation of chemical and physical transformations (especially in manufacturing vessels exclusively penetrable by neutrons).

Revolutionizing Computing Technologies

(also reference the Quantum Science chapter)

The rising demand for data storage and computation threatens to consume up to 10 % of global electricity in the coming decades. Paradigm-shifting technologies, such as neuromorphic computing and quantum materials, require breakthroughs in materials science and chemistry:

- Neuromorphic Computing: Mimicking the low-power architectures of the human brain using nanoionic memristors and ion-gated transistors [6]. Neutron spectroscopy at STS can elucidate ion transport and dynamics critical for advancing these materials.
- Quantum Materials: Developing next-generation data storage technologies will depend on understanding the structure and behavior of metastable phases and dynamic interfaces.

3.1.2.2 Relevance to STS

Addressing these challenges demands advanced material characterization tools capable of probing complex systems under real-world conditions. The STS will provide:

- *In-situ* and *Operando* Capabilities: Investigating materials and processes in their functional environments, such as chemical reactors or geological storage systems.
- Time-Resolved Insights: Probing dynamics across timescales from femtoseconds to seconds, critical for understanding processes like catalysis, ion transport, and reaction kinetics.
- Integration of Imaging and Diffraction: Simultaneously resolving structural, chemical, and dynamical properties to optimize material design and process efficiency.

By enabling groundbreaking discoveries in sustainable chemistry, STS will accelerate the transition to net-zero emissions, circular material flows, and energy-efficient industrial systems

3.1.3 Food, Water, and Resource Resilience

Grand Challenge. Ensuring the security, availability, and sustainability of water, food, and critical terrestrial resources is an urgent global priority. The interdependence of these essential systems—known as the food-energy-water-resource nexus—is under increasing strain due to climate change, population growth, and resource depletion. Addressing these challenges requires transformative technologies, innovative materials, and multidisciplinary approaches to secure a sustainable future.

3.1.3.1 Scientific and Technological Impact

Agriculture

Global agricultural productivity depends heavily on synthetic nitrogen and phosphorus fertilizers. The Haber-Bosch process, which synthesizes ammonia fertilizer by enabling atmospheric nitrogen to react with hydrogen, consumes approximately 2% of global energy and emits ~310 megatons of CO_2 annually.

Modern ammonia production requires a staggering 29.7 million BTUs of net energy per ton of nitrogen [11, 12].

Phosphorus, primarily derived from finite phosphorite ores, also faces sustainability challenges. Only about 20 % of phosphorus used in agriculture enters the human diet, with the rest lost to soils or waterways. In soils, phosphorus is often chemically bound and bio-inaccessible, contributing to nutrient runoff, eutrophication, and harmful algal blooms in water bodies. To enhance food security and sustainability, we must develop systems to recover, recycle, and reuse phosphorus efficiently. This includes designing materials and processes that enhance bioavailability and improve nutrient uptake in plants. Neutron scattering and imaging techniques at the STS will provide critical insights into phosphorus dynamics in soil-plant systems, helping design strategies to minimize environmental impacts.

Water

- **Geological Importance of Water**

Water plays a critical role in shaping Earth's geologic features and supporting ecosystem functions. Below the surface, water-rock interactions influence the formation and stability of aquifers, while at the surface, water erosion, deposition, and solute transport are key to nutrient cycling. Understanding these processes at molecular and nanometer scales is vital for predicting ecosystem responses to environmental stressors such as climate change, pollution, and over-extraction

- **Drinking Water Challenges**

Access to clean drinking water remains a global challenge. Desalination, while promising, is energy-intensive and requires advanced materials to improve efficiency. Technologies that mitigate impurities like volatile organic compounds (VOCs), heavy metals, and emerging contaminants are essential for maintaining water quality. Novel porous materials, such as graphene-based membranes and MOFs, show great promise for achieving high selectivity and low-energy purification. Neutron imaging and scattering at the STS can enable real-time monitoring of filtration processes, offering valuable insights into the design and optimization of these materials for scalable water treatment solutions.

- **Watershed and Soil Systems**

At watershed scales, ecosystems respond to solute gradients and micro-scale interactions [13, 14]. Soil, a highly heterogeneous matrix, controls the long-term fate of carbon, nutrients, trace elements, and contaminants. Its intricate network of pores and aggregates governs water flow and microbial activity, shaping nutrient and solute availability. Neutron techniques can probe these complex systems at scales ranging from nanometers to meters, enabling detailed studies of soil-water-plant interactions and their implications for water retention, nutrient cycling, and carbon sequestration [15, 16].

Critical Materials

- **Reservoir Rocks for Energy Storage and Carbon Sequestration**

The properties of reservoir rocks, such as mechanical strength, porosity, and connectivity, directly impact their capacity and stability for storing hydrogen, carbon dioxide, hydrocarbons, and natural gases. These properties are crucial for decision-making in alternative energy strategies and carbon sequestration. Advanced neutron imaging and scattering techniques can examine these rock systems under real-world conditions, shedding light on how fluid dynamics and chemical interactions affect their storage potential.

- **Raw Materials and Critical Elements**

The demand for critical elements like cobalt, lithium, and rare earth metals is rising rapidly due to their essential roles in renewable energy technologies, batteries, and electronics. However, mining these materials poses significant environmental and geopolitical challenges. Neutron scattering can provide insights into the extraction and refinement processes by investigating the structural and dynamic properties of mineral ores, improving efficiency while reducing environmental impact. Additionally, advancements in recycling and recovery technologies for these critical elements will benefit from neutron-based studies of material degradation and reusability.

3.1.3.2 Relevance to STS

The penetrating nature of neutron beams offers a distinct advantage in studying the internal structures and dynamics of geological and environmental materials, enabling unparalleled insights into soil systems, reservoir rocks, and porous networks. Soil systems are critical to the global carbon cycle and food production, yet their complexity—rooted in depth-dependent variations in composition, structure, and biological-abiotic interactions—poses a significant challenge. Porosity in soil aggregates, regolith, and reservoir rocks spans multiple scales, from sub-nanometer to millimeter-sized pores. Understanding the evolution of these pore networks and their influence on resource distribution, such as nutrient availability and water retention, is essential for predictive models of soil microbiome function and sustainability strategies.

Similarly, neutron studies are uniquely suited for unraveling the kinetics and mechanisms of environmental and engineered processes. These capabilities enable precise control and optimization of chemical and physical transformations, including catalysis, nucleation, self-assembly, degradation, and regeneration. Key applications include in-situ investigations of devices under operational stressors, efficient recovery of critical materials from electronic waste and contaminated sites, and the degradation of persistent pollutants such as microplastics (e.g., PFAS). Furthermore, neutron scattering can support innovative solutions for agricultural circular economies, such as phosphorus recovery and reuse, sustainable urban mining, and advanced water treatment systems.
The availability of multimodular systems at STS—allowing for controlled testing conditions and multimodal analyses—will be crucial for achieving a comprehensive

understanding of these complex processes. By integrating operando and in-situ observations with next-generation neutron instrumentation, STS can accelerate advancements in sustainable resource management and environmental resilience.

3.1.4 Need for the STS: Capabilities and Infrastructure

(note that this section can be removed or used to flesh out previous – why neutron sections)

Several themes cross-cut the challenges above that can be uniquely addressed by the characteristics of a brilliant cold neutron source with an optimized instrument suite. The cold neutrons, with an expected maximum at a wavelength of 5 Å, are the only efficient bulk probes available in this wavelength and suitable energy range. Therefore, they enable probing length scales from a few atomic diameters to macroscopic dimensions on the order of 100 micrometers and timescales from 10^{-12} to 10^{-5} s.

Neutron atom/isotope sensitivity. Neutrons are the preeminent tool to determine the physical and chemical state of the hydrogen atom. They provide great sensitivity to light atoms in the presence of heavier ones, and they enable studies where isotopic labeling is used to isolate a feature of interest. This sensitivity will be essential to chemistry and environmental grand challenges involving porous solids and membranes for separations, cathodes, anodes, and electrolytes for energy storage and electrochemical synthesis (eg. MOFs, polymer membranes, electrolytes, hydrogen storage materials, etc). Likewise, in many food and water-involved systems, the materials, chemicals, and molecules are primarily composed of light elements (e.g., C, O, H, P, and N), and the systems can be large and heterogeneous, e.g., the soil-plant microbiome and rhizosphere. The use of isotopes of O, P, and N in such experiments could enable essential tracking of nutrients, fostering the realization of a new understanding of nutrient uptake and starvation in plants. Large bandwidth cold neutrons from the STS are uniquely positioned to contribute to the needed structural and dynamical experimental data across these systems. Consideration for the simultaneous use of compact X-ray sources especially for imaging, would be extremely beneficial.

High brightness. *In situ* and *operando* experiments that probe the evolution of dynamic, functional systems under realistic operating or reaction conditions are essential to our ability to understand, predict, and control systems spanning catalysis, energy storage, and materials discovery and development. However, the ability to resolve changes in the materials on all the time scales relevant to their use and to interrogate systems with good spatial resolution is brightness limited. The world-leading brightness of the STS promises to transform both the time scale and spatial resolution of processes that can be evaluated. Small beam size will allow mapping of hierarchical structures in devices and natural systems. It also enables structural studies of single crystals that are of “X-ray size” (<<1 mm) and powders prepared in very small quantities using high-pressure presses and other synthetic approaches that cannot readily be scaled up. New experiment modalities may be achievable, including

3D imaging with scattering/spectroscopy providing chemical/structural insights within individual voxels. A new generation of compact sample environments, with smaller sample volumes that can facilitate rapid changes and uniformity in conditions, such as temperature and chemical environment will also be enabled by enhanced brightness. Responsive sample environments are a key enabler for the efficient deployment of AI-guided experiments, as they can accommodate dramatic changes in conditions on time scales that are fast relative to the changes in the material system. Examples of sustainability systems that could benefit from such characterization include pharmaceuticals, MOFs, nanoparticles/nanocrystals (organic, inorganic, alloys, hybrids, aggregates), and a wide range of soft materials (biomaterials, biomolecules, micelles, polymers).

Multimodal. The grand challenges in sustainability introduced above represent many system-level science and engineering problems, often involving complex, hierarchical, and dynamic chemical and physical processes across many length and time scales. To solve such problems, we must leave behind bespoke neutron instruments optimized to probe narrow windows of energy or length scale and, by corollary, narrowly constrained experiments designed to isolate conditions or processes addressing a single scientific hypothesis. The source and instruments at the STS will provide game-changing advances in the study of the food-energy-water systems by enabling the study of complex systems in or approaching their natural/operating states.

Neutron scattering is ideally suited for statistically characterizing pore networks and their evolution over a wide range in length-scales (Zachara et al. 2016). Scattering techniques such as SANS/USANS have been used to interrogate the pore network structure in rocks, regolith, and soils. For example, the pore network present in native and weathered Marcellus shale samples reveal drastic changes in porosity and pore size distribution with weathering present both in the finest and the largest pore fractions (Anovitz and Cole 2015). However, the combination of long measurement times and the need to combine two techniques (i.e., SANS and USANS) to cover the length scales desired limits our ability to describe the pore network in sufficient detail. Combining imaging/tomography and SANS would provide the most impact in this field. Being able to measure the dynamics of atoms and molecules at interfaces gives insight into almost every critical chemical process, from catalysis, mechanochemistry, CO_2 CCUS, water transport, and cross-membrane diffusion to interactions in molten salts. The high brightness and high-count rate potential of instruments at the STS will allow unprecedented inclusion of structure-*dynamics*-function consideration in developing more efficient and useful materials and processes.

Multi-modal beamlines (spanning lengths, time scales, and/or dynamics), equipped with suitable sample environments will be capable of isolating the composition, nature, location, and behavior of key H, Li, C, N, P, and other light element-containing species as they function and interact within both engineered systems such as fuel cells, batteries, and chemical reactors, and natural systems such as subsurface geological formations, root systems, soils, exoplanet interiors, etc. In-situ and operando neutron experiments to probe chemical reactivity and structural changes dependent upon guest partial pressure, temperature, irradiation, magnetic/electric field/etc. will be crucial.

Materials discovery and synthesis exploration. Computational scientists can predict high-performance, next-generation materials with the potential to revolutionize energy technologies. However, they cannot predict the synthesis paths required to realize these hypothetical materials. This limitation arises from the complex, dynamic, and non-equilibrium processes involved in material synthesis, which span multiple length, energy, and time scales. For example, in solution-phase synthesis, the assembly of ions and molecules and stabilizing different phases or structural motifs depends on interactions between solvent molecules (e.g., water), ions, and other structure-directing agents at the surface of the nascent nuclei/nanoparticles. These interactions play a crucial role in determining the evolution of the reaction and the structure/phase of the ultimate product. The small, brilliant neutron beams provided by STS open the possibility of probing these reaction pathways with time resolutions matched to the synthesis reaction time scales. The differentiated elemental sensitivity of neutrons will allow us to directly observe how water, ions, and structure-directing agents influence the reaction process, leading to a predictive understanding of synthesis science and accelerating the discovery of revolutionary new materials. E.g. https://doi.org/10.1021/acsmaterialslett.1c00193

Active-adaptive-autonomous control. The STS-wide emphasis on integrating modeling and simulation with data acquisition will flip the paradigm of acquire-then-analyze in these fields, speeding up the time to discovery and dissemination of new understanding. It will be possible, for example, to map spectral features to their molecular origins in real time. This will be enhanced by 'digital twins' of experiments, deployed to optimize planning all the way from estimating beam conditions, required run times, and necessary sample qualities, to evaluating data processing strategies, ancillary resource requirements, and instrument configurations. Connecting modular sample environment and control systems capable of manipulating measurement conditions with external stimuli (i.e., temperature, pressure, and the inclusion of fluid, magnetic field, and electrochemistry) will enable smart active-adaptive-autonomous experimentation, harnessing data needed to inform models and evaluate wholistic new solutions more rapidly and efficiently than ever before. The integration of *active-adaptive-autonomous control feedback mechanisms* provides a transformative pathway for steering complex experiments in real-time, for example, within systems containing water. Utilizing real-time data and adaptive algorithms, these control systems can dynamically respond to varying experimental conditions and challenges, ensuring just-in-time decision making and optimal resource allocation. Through this innovative approach, we can achieve semi-automated experiments management, crucial for addressing the growing demand of large and critical data collection (i.e. detailed analysis of water's behavior and interactions in natural and engineered systems). Integrated computing infrastructure and AI/ML algorithms at STS will enable users to map existing knowledge bases of the material, such as structural and dynamical information, onto neutron scattering event data streams in real-time, facilitating immediate comparison through a digital-twin system. This capability allows for on-the-fly calibration, alignment, anomaly and feature detection and interpretation, and autonomous experiment steering. Coupled with high brightness and small sample sizes, and other techniques such as pump-probe, this approach will unlock critical insights into chemical reactions and transport processes that only neutrons can probe, with unprecedented spatial and temporal resolution. With built-in “learning” capabilities, instruments at STS can be trained to continuously improve over time, making future experiments more efficient, or even suggest new systems to study for accelerated materials discovery. By harnessing the power of AI, ML, and advanced computing, as well as the leadership computing facilities at ORNL, STS can significantly enhance its scientific capabilities and accelerate the pace of discovery across multiple fields.

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