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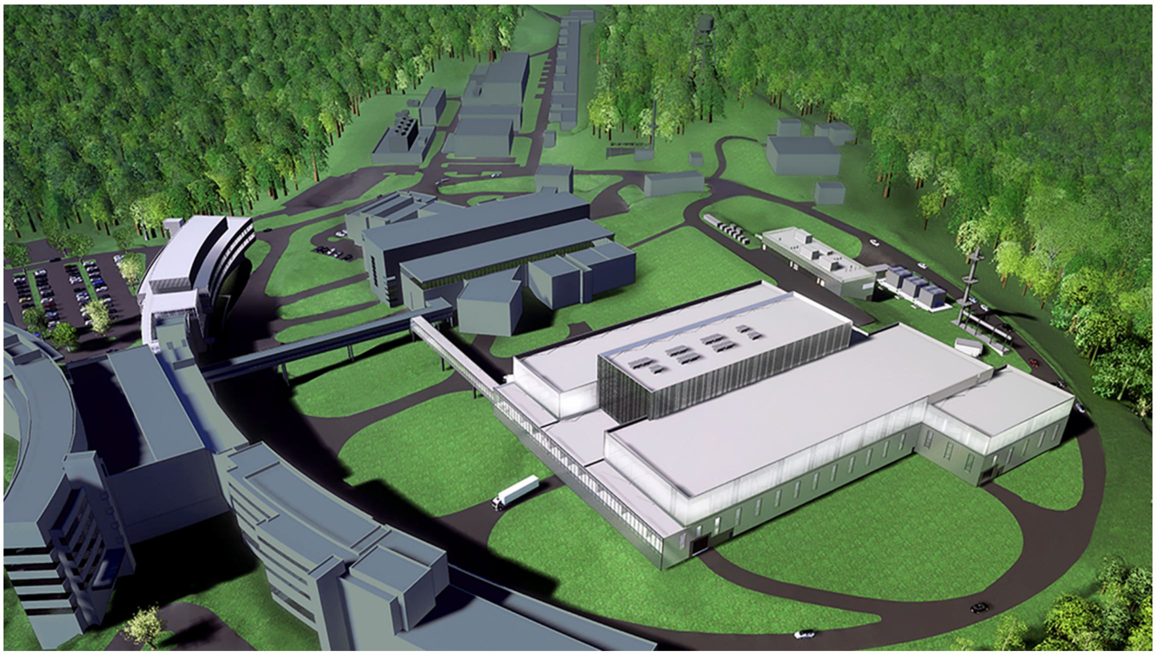
Second Target Station Project: STS Cross-Directorate Workshop on Hydrogen Fuel



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July 2024

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STS Cross-Directorate on Hydrogen Fuel

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ACRONYMS

AEM	Alkaline Exchange Membrane
AEM	Anion Exchange Membrane
AWE	Alkaline Water Electrolysis
AI	Artificial Intelligence
DOE	Department of Energy
ESTD	Energy Science and Technology Directorate
FTS	First Target Station
HTHA	High-Temperature Hydrogen Attack
INS	Inelastic Neutron Scattering
MEA	Membrane Electrode Assembly
MOF	Metal-Organic Frameworks
NR	Neutron Reflectometry
NScD	Neutron Sciences Directorate
NSE	Neutron Spin Echo
ORNL	Oak Ridge National Laboratory
PFSA	Perfluorosulfonic Acid
PEM	Proton Exchange Membrane
PSD	Physical Sciences Directorate
QENS	Quasi-Elastic Neutron Scattering
SANS	Small Angle Neutron Scattering
SE	Sample Environment
SNS	Spallation Neutron Source
STS	Second Target Station

1. EXECUTIVE SUMMARY

Hydrogen, particularly green hydrogen produced through electrolysis using renewable energy, is poised to play a critical role in decarbonizing the global economy. Its ability to address the intermittency of renewable energy sources and decarbonize hard-to-electrify sectors positions it as a vital component of a sustainable energy future. Interest in hydrogen as a clean energy carrier is in a decade of unprecedented growth, with dozens of countries having released national hydrogen strategies contributing to a global hydrogen economy [1]. In 2021, the Department of Energy (DOE) announced the Hydrogen Shot, the first of the Energy Earthshot Initiatives, which aims to lower the cost of clean hydrogen to $1/kg by 2031 [2]. This initiative was followed by a considerable increase in funding for hydrogen technologies through the Bipartisan Infrastructure Law (BIL), with $8 billion recently announced for regional demonstration projects (Hydrogen Hubs) and another $1.5 billion aimed at research and development of electrolyzers, fuel cells, manufacturing, and recycling [3]. The 2023 U.S. National Clean Hydrogen Strategy and Roadmap identifies the cost of clean hydrogen as a critical challenge for achieving economic scale. This includes the cost of hydrogen production by electrolysis, delivery and dispensing, onboard storage, and end-use technologies like fuel cells. Fundamental research and development into catalysts, component architectures, and material durability are critical to lower the costs of these vital technologies aimed at achieving a net-zero carbon emission economy by 2050 [4, 5].

This report highlights the discussions and outcomes of a cross-directorate workshop on how neutron instruments at the planned second target station (STS) can accelerate research in hydrogen technologies, outlining broad scientific possibilities enabled by STS. The document provides brief descriptions of various experimental approaches, both existing and those under development. However, it is not intended to be a comprehensive list of all instrumentation needs or a detailed instrument design plan. The STS planning process will balance scientific opportunities, impact, instrumentation requirements, available resources, and infrastructure for a balanced approach. This document serves to inform that process. The workshop, which was held at Oak Ridge National Laboratory (ORNL) on January 30th, 2024, brought together ORNL scientists from the STS Project, the Physical Sciences Directorate (PSD), the Energy Science and Technology Directorate (ESTD), and the Neutron Sciences Directorate (NScD).

The workshop featured presentations on the current trends and challenges in clean hydrogen technologies, divided into three categories: production, storage, and utilization. Presentations by scientists engaged in the planning and designing of the STS instrumentation enabled fruitful discussion on how these instruments could be utilized to solve some of the critical challenges for hydrogen technologies.

STS instruments will revolutionize neutron scattering capabilities for US scientists [6], dramatically accelerating the discovery of new materials and developing devices crucial for a sustainable hydrogen economy [5, 7]. Neutrons are suited to address the critical challenges of hydrogen systems with unique sensitivity to light elements, heterogeneities, and dynamics. Unlike X-rays and electrons, neutrons are more sensitive to light elements like hydrogen, a crucial component in hydrogen technologies. Neutron scattering excels at studying complex, multi-scale, heterogeneous materials due to its sensitivity to variations within the materials. Neutron scattering covers extensive time scales relevant to condensed matter, from femtoseconds to days and beyond.

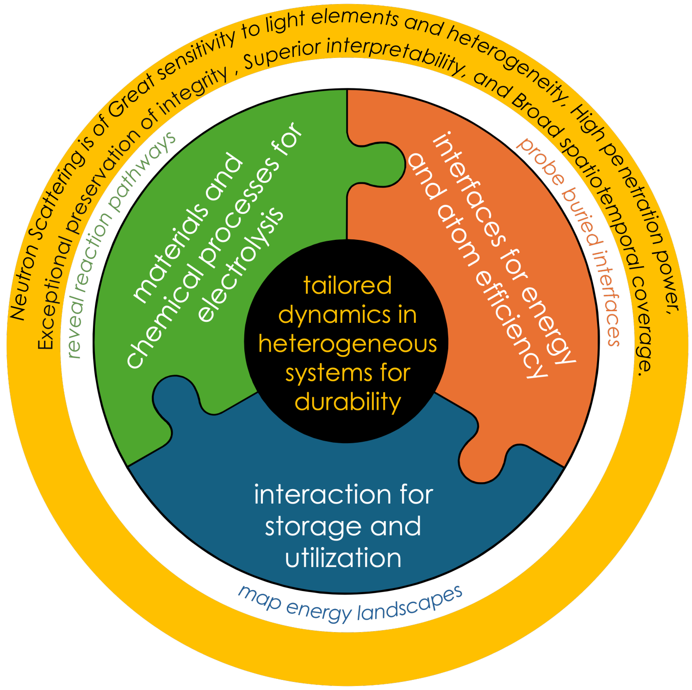

Figure 1 Research opportunities and unique advantages of neutron scattering for H2 @ scale.

The weak neutron-matter interactions allow neutrons to penetrate deeply to perform operando experiments in realistic environments. This weak interaction also leads to high data interpretability, resulting in clearer, more reliable conclusions even with sophisticated models. Neutrons are gentle probes, preserving samples' integrity during experiments. As shown in Fig. 1, these characteristics enable neutron scattering to be an indispensable tool for researchers to seize the scientific opportunities for hydrogen at scale [5]:

- Neutron scattering visualizes reaction pathways: It allows us to see the fundamental steps involved in materials and chemical processes for electrolysis, providing crucial insights for optimization.
- Neutron scattering probes buried interfaces: It can analyze hidden interfaces within heterogeneous materials, opening doors to greater energy and fuel efficiency.
- Neutron scattering maps the energy landscape: It provides accurate information on the interactions within materials, leading to breakthroughs in hydrogen storage and utilization technologies.

Conventional neutron scattering usually studies a single-component sample in equilibrium. However, the inherent complexities and multi-scale nature of hydrogen systems, characterized by their multicomponent structures and dynamic temporal and spatial variations, necessitate a paradigm shift in neutron scattering experiments, as illustrated in Fig. 2. A synergistic and integrated approach is crucial, seamlessly combining operando environments, multimodal characterization, and multiscale computational modeling. To achieve these goals, STS instrument design aims to:

- Develop in-situ and operando environments to study non-equilibrium systems.
- Enable multimodal characterization on a system to achieve a holistic view, connecting structure and dynamics and probing extended spatial and temporal scales.
- Implement advanced computational and data science tools.
- Incorporate robotics to enable Artificial Intelligence (AI)-assisted experimental steering and autonomous capabilities.

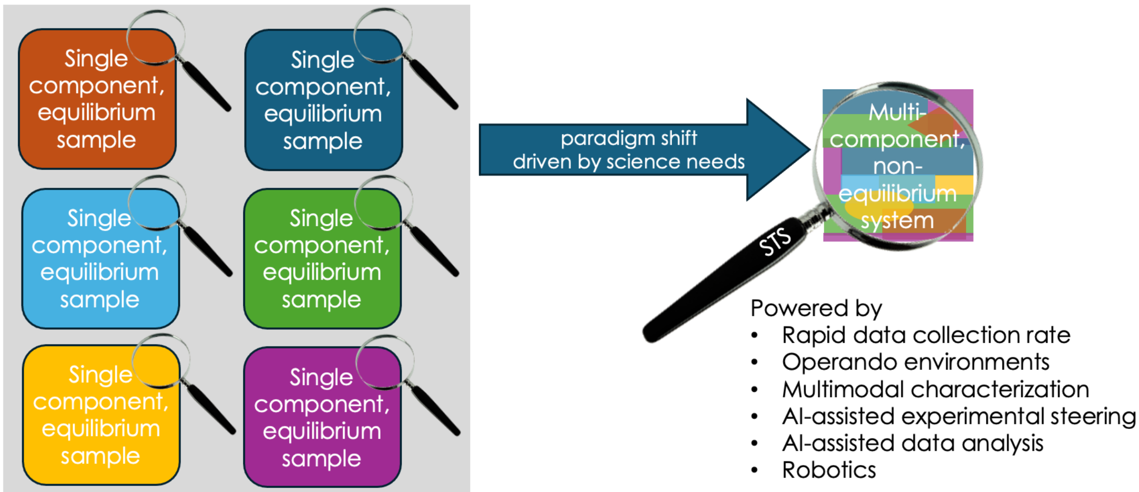

Figure 2 Conventional neutron scattering usually studies a single component, an equilibrium sample. The multi-component structures and dynamic natures of complex hydrogen systems will drive a paradigm shift in the experimental approach. STS instruments will pioneer this shift through much faster data collection data, operando environments, multimodal characterization, AI-assisted experimental steering and data analysis, and high-level automation using robotics.

This paradigm shift aims to establish a robust framework that can accurately predict and elucidate the intricate interplay of various phenomena within these systems, paving the way for the development of efficient, durable, and scalable hydrogen technologies. **This presents significant opportunities for STS to contribute to the hydrogen economy transformation, with two orders of magnitude faster data collection, realistic operando environments, multimodal probes, AI-assisted experimental steering and data analysis, and advanced automation using robotics.**

2. STATUS AND CHALLENGES FOR HYDROGEN TECHNOLOGIES

The vision of DOE's H_2@Scale initiative, schematically illustrated in Figure 3, is to expand hydrogen from its current centralized use in the oil refining and ammonia industries to a flexible energy carrier used in multiple sectors including transportation, liquid fuels (e.g., biofuels, synfuels), heat generation, and energy storage. Multiple offices and programs across DOE are working together to develop cost-effective production methods, establish reliable transportation and distribution infrastructure, find efficient storage solutions, adapt existing infrastructure, and expand hydrogen applications across various sectors. Hydrogen can be produced from natural gas, coal, nuclear, and renewables, serving as a critical feedstock for multiple industries. When produced by renewable-powered electrolysis or coupled with carbon capture, hydrogen production enables zero or near-zero emissions in numerous applications and acts as a "responsive load" on the electric grid, supporting large-scale and long-term energy storage. Hydrogen as an energy carrier has many end uses, including in ammonia production and steel refining. It can also produce synthetic fuels from captured CO_2 or electricity by a proton exchange membrane (PEM) fuel cell. Fuel cells are under intense development for heavy-duty transportation, including Class 8 tracks, trains, ferries, and airplanes [8].

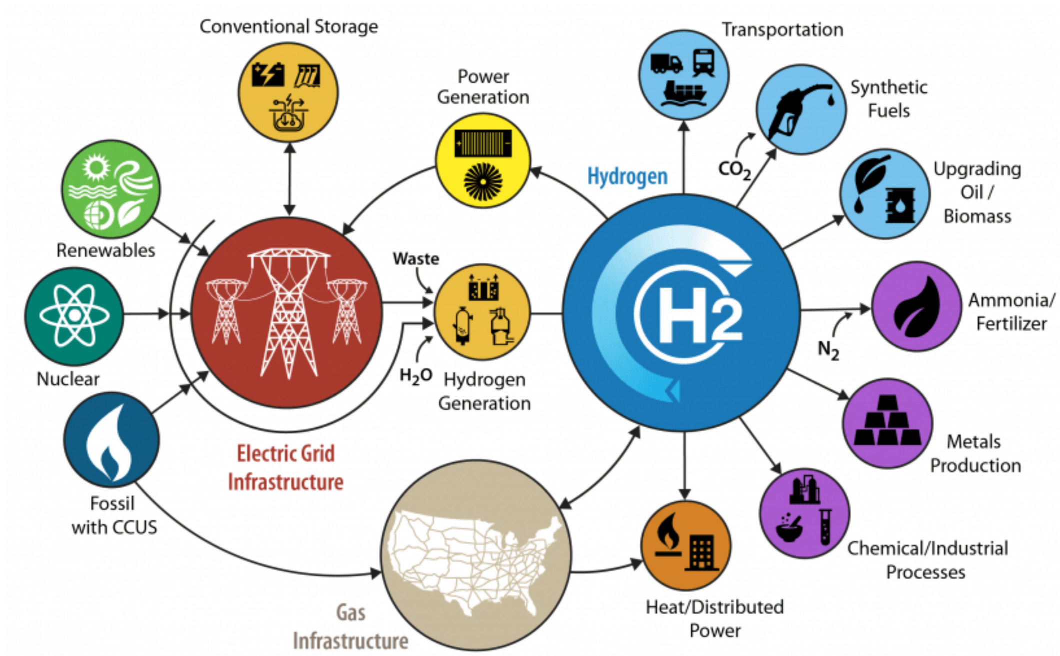

Figure 3 H_2@Scale is a U.S. DOE initiative to make hydrogen production, delivery, storage, and use more affordable and cleaner. (https://www.energy.gov/eere/fuelcells/h2scale)

To pave the way for a future where clean hydrogen can be a viable energy carrier, we must overcome the current limitations in hydrogen production, storage, and utilization. These advancements should include water splitting, catalytic or thermal methane cracking, microbial production under mild conditions, and extraction from diverse feedstocks such as biomass and waste. Additionally, we must explore new material- and chemical-based strategies to ensure the safe and efficient delivery and storage of hydrogen. The scope of carbon-neutral hydrogen must encompass energy-intensive sectors, including transportation, power generation, and industrial processing.

A comprehensive understanding of molecular-level mechanisms is essential to facilitate these advancements. We must transform experimental techniques incorporating advanced data science and AI approaches and develop predictive/prescriptive theoretical modeling. This transformation will foster the synthesis of innovative materials and chemicals, deepen insights into hydrogen interactions, elucidate the dynamics of complex interfaces, and offer pathways to mitigate critical degradation processes. As articulated in the DOE Basic Energy Sciences Roundtable reports [5], vital scientific questions on carbon-neutral hydrogen technologies include:

- *How do we codesign multiple components that work together to enable stable, efficient electrolysis for carbon-free production of hydrogen from water?*
- *What fundamental insights are needed to control and selectively tune hydrogen interactions with molecules and materials?*
- *How can interacting, evolving interfaces be tailored at multiple length scales and timescales to achieve energy-efficient, selective processes and enable carbon-neutral hydrogen technologies?*
- *How can we identify and understand the complex mechanisms of degradation to obtain foundational knowledge that enables the predictive design of robust hydrogen systems?*

The workshop discussion highlighted these topics, a synopsis of which is given below.

2.1 ELECTROLYSIS FOR HYDROGEN PRODUCTION

Electrolysis is a promising technology for carbon-neutral hydrogen production. However, significant advancements are needed to reduce capital costs and improve electrolyzer efficiency and durability. This includes optimizing the composition and performance of membranes, catalysts, and electrode layers and developing a deeper understanding of reaction mechanisms and degradation processes in different operating environments.

Besides water electrolysis, producing hydrogen fuel from sunlight and water, two of Earth's most abundant natural resources, represents one of the most promising pathways for carbon neutrality. Several encouraging approaches to scalable solar water splitting exist, e.g., photochemical, photoelectrochemical, and photovoltaic electrolysis systems. However, none of these approaches are presently comparable with today's electrolysis technologies in an economically viable way. Competitive solar-based hydrogen production will require cost reduction. One critical step is to revolutionize the rational design of the material with high photoactivity to improve solar-to-hydrogen efficiency for hydrogen generation from water splitting [9, 10]. In recent years, investigating the issue of the trade-off between material impurity and device performance has drawn much attention from researchers [11]. Despite noted improvement in the performance of impurity-doped materials, the mechanism by which this improvement is brought about and the exact role that hydrogen plays in these materials is still not fully understood.

2.2 HYDROGEN-MATTER INTERACTION

Efficiently storing and transporting hydrogen is crucial for a hydrogen-based energy economy. The low volumetric density of hydrogen necessitates innovative storage solutions beyond conventional compressed gas or cryogenic liquid methods. Developing material-based hydrogen storage, including adsorbents, metal hydrides, and liquid organic hydrogen carriers, is an active research area but faces challenges in achieving high hydrogen capacity, controlling the kinetics and thermodynamics of hydrogen uptake and release, and mitigating material degradation [12].

2.3 UNDERSTANDING AND CONTROLLING COMPLEX INTERFACES

Complex interfaces between different materials in hydrogen-generating systems present significant challenges for controlling reactivity and durability. A fundamental understanding of interfacial phenomena is crucial for optimizing performance and mitigating degradation in various hydrogen technologies, including electrolyzers, fuel cells, and storage systems. This requires developing advanced characterization techniques, multi-scale modeling frameworks, and innovative synthesis approaches to probe, predict, and control interfacial structures and dynamics.

2.4 MITIGATING DEGRADATION PROCESSES

Material degradation is a significant obstacle to the widespread deployment of hydrogen technologies. A lack of mechanistic understanding of degradation processes and their long timescales makes it challenging to design durable hydrogen systems. Developing in situ and operando characterization tools is needed to probe degradation mechanisms at the atomic level and degradation kinetics to identify structure-function relationships that govern material stability.

Understanding degradation mechanisms is challenging due to the simultaneous occurrence of multiple processes in complex hydrogen systems and their evolution over time. The conventional "top-down" approach, which involves studying real systems directly, often struggles to isolate individual mechanisms and establish accurate structure-function relationships. Neutron scattering experiments can adopt a "bottom-up" approach to study model systems with well-defined materials and interfaces, allowing for the systematic isolation and investigation of distinct degradation mechanisms. This approach enables a deeper mechanistic and energetic understanding and provides for controlled complexity, progressively building toward the intricacies of real-world hydrogen systems. Insights gained from model systems can guide the design of robust and durable materials for practical hydrogen applications.

3. WORKSHOP PRESENTATIONS

3.1 NEUTRON SCATTERING FOR HYDROGEN SCIENCE

The first session of the workshop started with an overview of the Second Target Station project, followed by presentations on new capabilities of the initial 8 instruments, covering a broad spectrum of scattering techniques, from reflectometry (QIKR [13]), imagining (CUPI^{2}D [14]), small/wide angle scattering (CENTAUR [15]), diffraction (PIONEER [16] and VERDI [17]), and spectroscopy (BWAVE [18], CHESS [19], EXPANSE [20]).

Due to its unique sensitivity to hydrogen, neutron scattering is a powerful tool for studying hydrogen-containing materials. While X-rays and electrons are well-suited for investigating materials with high atomic weights, neutron scattering offers advantages in probing lighter elements. This complementary nature allows researchers to obtain a more comprehensive understanding of materials and processes in hydrogen systems. Neutron scattering techniques can provide crucial insights into structure, dynamics, and hydrogen interactions within materials. For example, INS can directly measure the excitations of H_2 as a quantum rotor due to its high sensitivity to its local structural and chemical environment. With modern data analysis tools, INS is ideal for understanding the hydrogen-matter interactions, especially for H_2 deep inside bulk materials. A few scientific applications are given below.

Characterizing Hydrogen Storage Materials: Neutron scattering techniques can be used to probe the interactions of hydrogen with materials designed for storage applications [21]. It helps determine the binding energies, binding sites, diffusion properties, and the role of steric hindrance in the adsorption and desorption processes. This information can guide the design of more efficient hydrogen storage materials. For example, neutron diffraction can help understand how hydrogen behaves within metal-organic frameworks (MOFs) [22-24], promising materials for adsorptive hydrogen storage. By analyzing real-space pair distribution functions, total neutron scattering can even provide the locations and bonding of D/H in amorphous and disordered materials [25]. Inelastic neutron scattering (INS) has the advantage that it is free from optical selection rules, probes beyond the center of the Brillouin zone, and can be accurately modeled. Combined with Density Function Theory, INS provides direct information on the nature of the interaction of hydrogen with matter [21, 26].

Studying Catalysts and Revealing Reaction Pathways: Neutron scattering techniques help study catalysts [27, 28]. Experiments under operando conditions will allow researchers to observe real-time reaction pathways [29]. Identifying rate-limiting steps in a reaction can help researchers design more effective catalysts by focusing on materials and structures that overcome those limitations. Similarly, understanding how catalyst deactivation occurs allows for developing strategies to prolong the catalyst. Neutron radiography and tomography have been used to study the water distribution and flow within operating fuel cells [30, 31]. Since water is a byproduct of the reaction in fuel cells and neutrons' sensitivity to hydrogen, these techniques can provide valuable information about the performance and operation of fuel cells.

Probing Heterostructure Phenomena: Neutron scattering provides valuable insights into the complex interfaces in hydrogen systems, especially those involving soft materials like polymers. It can characterize how ionomers and membrane electrolytes change at the atomic level during fuel cell or electrolysis operation [32], helping understand how degradation impacts proton transport. Notably, neutron scattering effectively resolves the structure of ionomers in catalyst-ionomer composite electrodes and how the catalyst-ionomer interface changes during electrochemical processes that contribute to performance degradation [33].

Operando Studies of Degradation: Neutron scattering, being non-destructive, allows for operando studies, where materials are investigated in real-time under operating conditions. This is particularly valuable for studying degradation processes, which often occur slowly over long periods. For instance, neutron scattering can track changes in the structure and dynamics of a fuel cell membrane as it degrades during operation [29], offering insights into the mechanisms and factors influencing degradation.

Other novel applications exist. Hydrogen embrittlement begins at ppm-level hydrogen concentrations [34], making it difficult to probe the existence of hydrogen directly. However, incoherent neutron scattering combined with diffraction analysis has been used to nondestructively detect hydrogen embrittlement at low hydrogen concentrations in high-strength steel [35].

3.2 SCIENCE OPPORTUNITIES FOR THE HYDROGEN ECONOMY

The workshop's second session started with an overview of ORNL hydrogen strategy by Dr. Vivek Sujan, followed by several talks on various aspects of hydrogen science, including production, storage/transport, and utilization. Sujan’s talk highlighted ORNL's aspirational vision of a broader coordinated R&D strategy in response to national efforts to accelerate the moves toward a hydrogen economy, a key component to achieving national decarbonization goals across various sectors of the economy. This coordinated R&D strategy would address challenges within the critical focus areas identified in the U.S. National Clean Hydrogen Strategy and Roadmap [4]. This strategy would leverage ORNL's core strengths and technologies to coordinate research and development efforts across different directorates. Neutron scattering, a key ORNL capability, is expected to play a significant role in catalysis, hydrogen storage materials, and degradation mechanisms. Below is an overview of the science talks.

3.2.1 Low-Temperature Water Electrolysis

Alexey Serov’s talk “Electrodes for Hydrogen Production: Supports, Catalysts and Additives” was devoted to ORNL’s involvement in several DOE funded consortia, such as Hydrogen from Next-generation Electrolyzers of Water (H2NEW), The Electrocatalysis (ElectroCat) Consortium and newly created Roll-2-Roll consortium. Primary components for building efficient, durable, and scalable electrodes are catalysts for electrochemical water splitting, which can be either precious metal-based (used in matured PEM systems) or completely free of Platinum Group Metals (used in emerging technologies based on Alkaline Exchange Membrane (AEM) and Alkaline Water Electrolysis (AWE) principles. Both families of materials have their advantages and disadvantages, mainly derived from an incomplete understanding of their electronic, crystallographic, and morphological properties. It was discussed that when using state-of-the-art iridium-based catalysts, a key R&D goal is to decrease the amount of this scarce, expensive, and domestically unavailable metal by alloying with less expensive elements. The rational design of such a complex, multimetallic system is currently in the early stages of development. Understanding the role of other dopants' role in the improvement of catalyst utilization or effect on the stability and durability can be dramatically accelerated by applying neutron scattering methods, such as Neutron Powder Diffraction, which provides additional information on the interaction of iridium with light elements, including hydrogen. For non-precious metal catalysts, there is a further complexity related to their amorphous structure. Conventional laboratory X-ray experiments are unsuitable for phase analysis, phase ratio, and Rietveld refinement for these cases, which can be achieved using neutron scattering methods.

Tom Zawodzinski’s presentation highlighted that current PEM electrolyzers rely on relatively thick perfluorosulfonic acid (PFSA) membranes, typically exceeding 100 µm. These PFSA membranes, like Nafion, have seen minimal evolution since the early 2000s. One of the notable challenges associated with PFSA membranes is their propensity to swell when exposed to water, exemplified by Nafion membranes expanding by 50-100% when fully hydrated. This swelling necessitates thicker membranes in electrolyzers, consequently leading to efficiency losses.

Moreover, the influence of swelling on membrane strength under compressive and tensile loads remains inadequately understood, partly due to the limited tools available for accurately measuring membrane swelling in liquid water. Developing non-PFSA membrane materials with reduced susceptibility to swelling is, therefore, pivotal for enhancing the efficiency and durability of PEM electrolyzers.

Xiao-guan Sun's presentation highlighted novel alkaline exchange membranes (AEMs) for hydrogen production, aligning with the increasing global demand for green hydrogen and the DOE's objective to reduce clean hydrogen costs. The presentation emphasized the cost advantages of AEMs, stemming from non-noble metal catalysts and cheaper hydrocarbon membranes. This shift in materials notably allows for transitioning from titanium to stainless steel, reducing stack part costs by 75%. Moreover, AEMs can enhance the kinetics of oxygen reduction reactions. However, the presentation acknowledged that AEMs require further development, particularly in improving their stability and ionic conductivity. Stability is crucial for practical applications. Optimizing the AEM structure and reducing membrane thickness are critical strategies for enhancing stability. The presentation concludes by exploring the potential of neutron scattering techniques for AEM structural optimization. Can neutrons reveal the formation of fast ion transport channels? How can we differentiate between two possible ion transport mechanisms: molecular diffusion and structural diffusion? Can these experiments be done without deuteration?

3.2.2 Hydrogen Storage

In a talk by Jun Yang, materials-based hydrogen storage is reviewed. Converting generated hydrogen (H_2) into liquid fuels or other chemicals offers a solution for easier transportation. Jun compared the advantages and disadvantages of various storage systems, including conventional and complex hydrides, sorbents, and chemical hydrides. The discussion covered material preparation, characterization methods, and the challenges associated with each type. The talk also included a few instances where neutron scattering offers valuable insights into the fundamental mechanisms. Neutron diffraction can pinpoint the location of hydrogen (or deuterium) atoms within metal hydrides, enabling optimization for maximum storage capacity. Neutron scattering methods can also elucidate reaction mechanisms in complex hydrides, advancing the understanding of their reversibility and minimizing side effects. Neutron scattering and spectroscopy can characterize the interaction of hydrogen with sorbents, distinguishing between molecular and atomic hydrogen. Finally, it can assist in catalyst selection and shed light on catalytic reaction mechanisms.

Zhili Feng discussed the compatibility of engineering structural materials used for hydrogen storage. Feng highlighted two long-standing challenges: (1) hydrogen embrittlement of steels and metallic alloys and (2) high-temperature hydrogen attack (HTHA). Studying hydrogen embrittlement with neutrons is difficult due to metals' low hydrogen (H2) concentration, typically ranging from 1 to 100 ppm. However, methane (CH_4) formation offers an approach for investigating HTHA using various neutron scattering techniques. In-situ experiments that combine small and wide-angle scattering with tomography under temperature and stress can reveal the effects of CH_4 on the damage process across nano and micro-length scales. Additionally, neutron spectroscopy can provide insights into the dynamics of CH_4 formation under different conditions, including variations in alloy chemistry, microstructure, temperature, and pressure.

3.2.3 Low-Temperature Fuel Cells

The status and challenges of implementing hydrogen utilization in proton exchange membrane fuel cells (PEMFCs) for heavy-duty vehicle applications were presented in David Cullen's talk. In addition to battery vehicles, PEMFCs can play a critical role in decarbonizing the heavy-duty transportation sector, but fuel efficiency and component durability remain significant challenges to commercialization. Catalyst and ionomer materials development, manufacturing of novel electrode designs, and exploration of additives for mitigation degradation are key areas of ongoing research being addressed by the Million Mile Fuel Cell Truck Consortium (M2FCT). Neutron imaging of water management will be essential in integrating new electrode designs, and in situ, neutron scattering across a large Q range will be required to better understand ionomer-support-catalyst interactions that govern device efficiency and longevity.

Tomonori Saito introduced his work on phenyl-free quaternized vinyl-addition polynorbornene copolymers, which can be used for anion exchange membranes (AEMs), AEM fuel cells, and AEM electrolyzers. Polynorbornenes exhibit promising characteristics for use in fuel cells and electrolyzers. Notably, their excellent mechanical strength allows for fabricating thin membranes, as thin as 20 µm. These thin membranes, in turn, contribute to reduced area-specific resistance, a critical factor in fuel cell efficiency. Another key advantage is the conductivity of these polymers, exceeding 110 mS/cm at 80 °C in water. This high conductivity is attributed to the quaternization process, which introduces quaternary ammonium groups to the polymer structure, enabling efficient ion transport. Small-angle neutron scattering (SANS) analysis reveals that quaternized polynorbornenes exhibit distinct microphase separation when wet. This separation is crucial for creating pathways for ion conduction, thereby enhancing the overall conductivity of the membrane.

4. NEUTRON SCIENCE OPPORTUNITIES AT STS

4.1 NEW CAPABILITY NEEDS

Neutron scattering is an ideal tool to answer many critical H-related questions. Still, experiments are often infeasible at existing beamlines because of the small amount of sample volume or the low concentration of the substance of interest. The 20-100 higher flux available at STS beamlines will enable us to detect smaller samples and lower concentrations of H (or H_2) in samples, transforming our capability to study hydrogen science.

On the other hand, we must move beyond trial-and-error (Edisonian) approaches and adopt a combination of predictive theoretical modeling and advanced experimental techniques to accelerate the development of hydrogen technologies to meet energy and environmental needs. While neutron scattering is essential, there are currently limitations in their application to complex hydrogen systems (Fig. 4). To bridge this capability gap, advancements are needed in operando environments, multimodal characterization methods, powerful data analysis tools, and robotic integration for automation and AI-assisted experimental steering. These developments will unlock the full potential of neutron scattering instruments, enabling them to meet the critical scientific needs of hydrogen research. STS instruments will take full advantage of these developments, bridging the gap between the need for hydrogen science and neutron scattering capabilities.

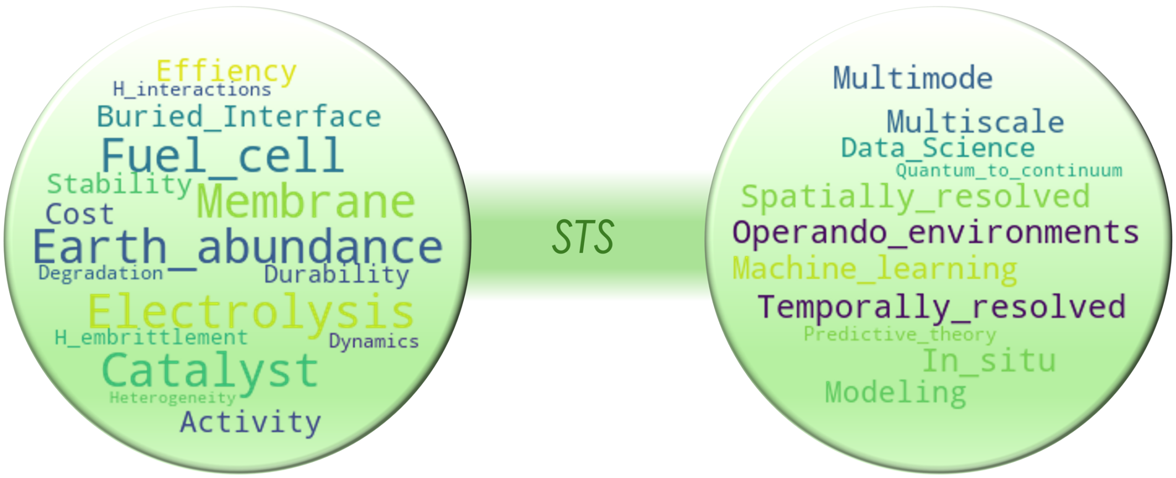

Figure 4 STS bridges the gap between H2 @ scale challenges and advanced methodologies through tailored instrumentation.

STS diffractometers bring new capabilities over FTS for studying hydrogen-rich materials. Their higher neutron flux, particularly for longer wavelengths, allows the analysis of dramatically smaller samples. Additionally, STS offers polarization analysis capabilities, a feature currently lacking in FTS but crucial for many studies. Furthermore, using smaller, thinner samples with STS reduces multiple scattering effects in hydrogen-rich systems. It allows the analysis of strongly neutron-absorbing materials, opening doors for research on promising materials like iridium-based hydrogen systems.

STS spectrometers offer a significant advantage with their higher neutron flux, enabling analysis of smaller samples, too. STS spectrometers can perform simultaneous INS and QENS measurements, eliminating variability caused by changing hydrogen content in traditional serial experiments. STS spectrometers with an open-table geometry will provide unprecedented access to high-resolution spectrometers, enabling optical probing and potentially valuable prompt-gamma analysis for various hydrogen systems. This open design also allows for future incorporation of stress/strain environments and even NMR analysis. Similar to diffraction, thinner samples facilitated by the higher flux can improve spectroscopic analysis of strongly absorbing materials like those in the iridium-based hydrogen family. For STS spectrometers with smaller samples, precise sample alignment will be a challenge, which is a critical aspect of successful experiments but often overlooked in neutron spectroscopy. Additionally, for comprehensive characterization, diffraction capabilities are essential to extend the benefits of consistent hydrogen loading to structural analysis, which is vital for concurrent modeling studies. The STS instrument design shall consider these challenges.

STS SANS instruments are highlighted by their capabilities to bridge the gap between atomic-level observations and larger-scale structural changes in materials like metals and semi-crystalline polymers. This is crucial for understanding both atomic ordering and nano-/meso-structure evolution. The superior time-resolved capability will be highly valuable for tracking structural changes over multi-length scales under operando conditions.

STS Spin Echo instruments will significantly improve the data collection rate, enabling routine access to measuring motions at the nanosecond scale. This capability is extraordinary for studying polymer electrolyte materials and the correlation between their segmental motions and hydrogen ion transport.

STS reflectometers will provide a "cinematic" operation in which the time-dependent evolution of interfaces can be recorded with unprecedented time resolution. In situ, neutron reflectometry (NR) has proven to be an excellent tool for studying the interfacial properties of energy conversion and storage materials. The interfacial properties of thin-film electrodes placed in specially designed electrochemical cells can be studied as a function of potential or state of charge at the nanometer scale [36].

STS image beamlines will combine direct and indirect imaging across a broad range of length and time scales. The instrument combines Bragg edge imaging and neutron grating interferometry. STS image beamlines will cover applications involving length scales from angstroms to micrometers and time scales from minutes to hours. Leveraging the high flux of cold neutrons from the high-brightness STS cylindrical moderator, they will support in situ and operando experiments.

On the other hand, workshop participants provided insights from user experiences and lessons learned at existing facilities, which will be crucial to designing STS instruments. The STS instrument should maintain a comprehensive suite of state-of-the-art sample environments, including existing capabilities like humidity control, high temperature, high pressure, and gas loading, and foster user engagement to develop new ones. Vapor deposition may be a more effective alternative to soaking whenever possible to minimize background noise from bulk fluids in surface-related scattering studies. The future operation shall revisit the operation model for efficiency and streamline the proposal review process to accommodate the fast pace of research better.

4.2 SCIENCE CASES

While neutron scattering has been a powerful tool for hydrogen science, instrument limitations have hindered the precise answers to some key scientific questions. The new capabilities of STS instruments promise to unlock a deeper understanding of fundamental mechanisms in this field. The following subsections will introduce a few examples.

4.2.1 Solar Water-Splitting

Recently, there has been an increasing interest in understanding the roles of material impurities in developing highly photoactive materials for efficient hydrogen production through water splitting [11]. For example, hydrogenated TiO_2, or black TiO_2, exhibited substantial solar-driven photocatalytic activities, including photo-oxidation of organic molecules in water and hydrogen production with a sacrificial reagent [37]. Similarly, many studies reported defect engineering in semiconductor metal oxides has demonstrated remarkable improvement in optical and electronic properties such as light absorption and charge separation [38-41], free-carrier concentration and conductivity, and ground-state energy structure [42].

TiO_2 stands out as a promising candidate due to its abundance, stability, and potential for further improvement. H-doping in rutile TiO_2 can induce an insulator-to-metal transition, boosting its photoactivity. However, the exact location and bonding of hydrogen atoms within the crystal structure, critical for this process, remain a mystery solely through theoretical calculations.

Neutron techniques offer a robust solution. Neutron diffraction directly reveals the local hydrogen structure and quantifies doping levels in treated TiO_2. Even more transformative, in-situ gas flow cell studies during annealing enable real-time observation of structural changes in small samples. INS spectroscopy provides further insights into hydrogen interactions and the local bonding environment. Additionally, NR allows for the investigation of treated TiO_2 thin films and interfacial structures at the nanoscale. STS will enable researchers to observe structural and compositional changes within the TiO_2 film by combining NR with increased data collection rates and in-situ/operando photo-electrochemical techniques. This spatial information is crucial for understanding the mechanisms behind enhanced photoactivity. Ultimately, neutrons can facilitate a comprehensive understanding of materials at both the atomic and macroscopic levels, leading to the design of efficient, durable, and cost-effective water electrolysis systems.

4.2.2 Catalysts

Operando neutron scattering at STS can unlock a new level of understanding in catalyst behavior for hydrogen science. Unlike other techniques, it allows researchers to probe dynamic changes in catalyst structure, composition, and behavior under real-world operating conditions. This capability is essential for unraveling the complexities of hydrogen interactions in hydrogen production, storage, and utilization. Also, neutrons are highly sensitive to hydrogen, making them ideal for studying these hydrogen-containing materials. This sensitivity provides valuable insights into how hydrogen adsorbs, diffuses, and reacts within catalysts. Researchers can gather crucial data to develop more efficient, stable, and cost-effective catalysts for various hydrogen applications by leveraging neutron scattering. For instance, as mentioned above, analyzing the elemental composition of NiFe-based catalysts for hydrogen production is challenging with traditional X-ray diffraction (Cu-Kα or Mo-Kα) due to limitations in distinguishing key elements. Neutron scattering offers a powerful solution for this specific challenge, especially considering that these complex oxi-hydroxides may have a different amount of hydrogen, being dynamically mobile under applied current. Having novel neutron scattering experimental setups will improve an understanding of catalyst behavior and accelerate the design of new materials.

4.2.3 Alkaline Exchange Membranes

AEMs offer advantages in hydrogen production, particularly green hydrogen, such as cost-effectiveness due to non-noble metal catalysts and cheaper membrane materials, including completely PFSA-free. AEMs also show the potential for improved kinetics in oxygen reduction/evolution reactions.

STS instruments can be utilized to optimize AEM structure. Neutron scattering can reveal the formation of fast ion transport channels by identifying local structural changes associated with channel formation through changes in diffraction patterns. Additionally, neutron scattering, specifically quasi-elastic neutron scattering (QENS), can help differentiate between two possible ion transport mechanisms: molecular diffusion and structural diffusion. QENS distinguishes these mechanisms based on the different characteristic energies involved in each. Isotopic substitution, using deuterium, can further enhance the differentiation. Molecular diffusion exhibits a strong isotope effect, implying that deuterium substitution significantly impacts its rate, whereas structural diffusion is less affected.

4.2.4 Time-Resolved Interfaces

Time-resolved NR unlocks a deeper understanding of interfacial electrochemistry and dynamic systems critical to various energy technologies. It provides a unique perspective on materials behavior under non-equilibrium conditions. Recent pioneering work at the Liquids Reflectometer (LR) at SNS First Target Station (FTS) has yielded valuable insights into electrochemical reactions. Blair et al.'s study on molybdenum cathode surfaces during nitrogen reduction and Candeago et al.'s investigation of solvation effects and ion valency at redox-polymer interfaces are prime examples [43, 44]. In these experiments, neutrons were continuously collected while a constant current was applied for extended durations (minutes to tens of minutes). The collected data was then retrospectively segmented into shorter intervals (15 seconds to 1 minute), generating a series of reflectivity profiles for analysis.

Striking a balance between time resolution and data quality per frame is essential for successful time-resolved experiments. The LR instrument's time resolution is limited by several factors, including relatively low neutron flux, inherent background noise, scattering contrast, detector efficiency, and associated electronics. With significantly higher neutron flux and modern design, STS reflectometers offer exciting possibilities for pushing the boundaries of time resolution in NR studies of electrolyzer and fuel cell devices.

4.2.5 Materials-Based Hydrogen Storage

Understanding how hydrogen interacts with materials is critical to developing efficient hydrogen storage technologies. Neutron scattering offers a unique advantage, providing insights into storage capacity, reaction mechanisms, and hydrogen adsorption behavior. Notably, it can pinpoint the location of hydrogen atoms within metal hydrides, revealing their maximum storage potential. In complex hydrides, neutron scattering helps unravel reaction mechanisms, allowing researchers to improve the reversibility of the storage process and minimize side effects. For sorbents, it clarifies how hydrogen adsorbs (molecules or atoms) – crucial information for selecting catalysts and understanding spillover phenomena, such as hydrogen storage on N-doped mesoporous carbon with a Ni catalyst. The high neutron flux at the STS instruments allows for the precise characterization of smaller samples and the investigation of kinetic pathways in complex systems under realistic conditions.

4.2.6 Materials Under Pressure

Due to neutrons' penetrating nature, neutron scattering techniques are particularly well-suited for studying hydrogen in materials under pressure. Neutrons can penetrate deeply into materials, including thick metal containers commonly used for high-pressure experiments. Many STS instruments will enable high beam flux with tunable sizes. Enhancing the signal-to-noise ratio isolates the desired material response from background interferences within the pressure cells. This allows researchers to extract accurate data from smaller amounts of samples under more complex and realistic conditions in high-pressure hydrogen tanks than is currently achievable.

4.2.7 Polymer Interactions

Neutron scattering offers researchers a powerful tool for understanding the intricate interactions between proton-conducting polymers, carbon support, and platinum within fuel cell systems. STS instruments will have enhanced data collection rates to support time-resolved studies with operando environments. This allows researchers to characterize material thickness and structure changes during operation and differentiate between fresh, degraded, and rebuilt polymer states, providing valuable insights into how degradation impacts these materials.

5. SUMMARY

Clean hydrogen is a viable energy carrier; however, we must overcome the current hydrogen production, storage, and utilization limitations. We shall prioritize carbon-neutral approaches and significantly enhance hydrogen production methods, develop new material- and chemical-based strategies to ensure the safe and efficient delivery and storage of hydrogen and gain an understanding of molecular-level mechanisms to enable predictive theoretical modeling. Many challenges exist to foster the synthesis of innovative materials and chemicals, deepen insights into hydrogen interactions, elucidate the dynamics of complex interfaces, and offer pathways to improve efficiency, reduce cost, and mitigate critical degradation processes.

Neutron scattering's unique sensitivities to light elements, heterogeneity, and dynamics provide great opportunities to address the challenges of hydrogen systems. Neutron scattering visualizes reaction pathways to see the fundamental steps involved in materials and chemical processes for electrolysis, providing crucial insights for optimization. Neutron scattering probes buried interfaces to analyze hidden boundaries within heterogeneous materials, opening doors to greater energy and atom efficiency. Neutron scattering maps the energy landscape to enable breakthroughs in hydrogen storage and utilization technologies. STS instruments will have much higher flux and broader spatiotemporal coverage, provide versatile, realistic environments, and incorporate data science and AI advancements. Through strategic advancements, STS instruments are projected to deliver performance exceeding existing instruments by two orders of magnitude. Such transformative capabilities will enable researchers to accelerate the discovery of new materials and develop devices crucial for a sustainable hydrogen economy.

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APPENDIX A: WORKSHOP AGENDA

STS Cross-Directorate Workshop on Hydrogen Fuel

8:30 am – 4:30 pm, January 30th, 2024

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Time (EDT)	Event	Speaker
8:30 - 8:40 am	Welcome and charge questions	Leighton Coates
Morning Session I: STS Instruments ***8:40 - 10:10 am Chair: Leighton Coates***		
8:40 - 9:10 am	STS Project Overview	Leighton Coates
9:10 - 9:25 am	STS Reflectometry and Imaging Capabilities - QIKR and CUPI^{2}D	John Ankner
9:25 - 9:40 am	STS Small Angle Scattering Capabilities – CENTAUR	Shuo Qian
9:40 - 9:55 am	STS Diffraction Capabilities – PIONEER and VERDI	Yaohua Liu
9:55 - 10:10 am	STS Spectroscopy Capabilities – BWAVES, CHESS and EXPANSE	Eugene Mamontov
10:10 - 10:30 am	Break	
Morning Session II: Science Talks ***10:30 am - 12:15 pm Chair: Hanyu Wang***		
10:30 - 10:45 am	ORNL Hydrogen Strategy Overview	Vivek Sujan
10:45 - 11:00 am	Understanding Components of Electrodes for Hydrogen Production: Supports, Catalysts and Additives	Alexey Serov
11:00 – 11:15 am	Hydrogen Production -2	Tom Zawodzinski
11:15 - 11:30 am	Materials-based Hydrogen Storage and Transportation	Jun Yang
11:30-11:45 am	Hydrogen Storage and Transport -2	Zhili Feng
11:45 am - 12:00 pm	Impact of Electrode Structure on Hydrogen Fuel Cell Performance and Durability	Dave Cullen
12:00 - 12:15 pm	Development of Novel Alkaline Exchange Membranes for Hydrogen Production	Xiao-Guang Sun

Lunch Talk		
12:15 -1:45 pm	Polyolefin-based Membranes and Ionomers for Hydrogen Fuel Cell and Electrolyzer	Tomonori Saito

Afternoon Breakout Sessions 1:45 - 4:40 pm (8600, C-156, C-152 and C-250)		
Time (EDT)	Event	Discussion Leader
1:45 - 2:40 pm	3 parallel breakout sessions – I *What are the emergent science problems regarding carbon-neutral hydrogen technologies that STS can address?*	1. Alexey Serov
		2. Dave Cullen
		3. Tom Zawodzinski
2:40 - 2:55 pm	Joint discussion and regroup	
2:55 - 3:00 pm	Break	
3:00 - 4:00 pm	3 parallel breakout sessions – II *How can we solve these problems using neutrons and the STS?*	1. John Anker and Yuxuan Zhang (Reflectometry, Imagining)
		2. Shuo Qian and Changwoo Do (Small Angle, Spin Echo)
		3. Yaohua Liu and Eugene Mamontov (Diffraction, Chemical Spectroscopy, Quasielastic Scattering)
4:00 - 4:30 pm	Joint discussion and summary	

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