Second Target Station Science Case

Presented to
Neutron Advisory Board

Presented by
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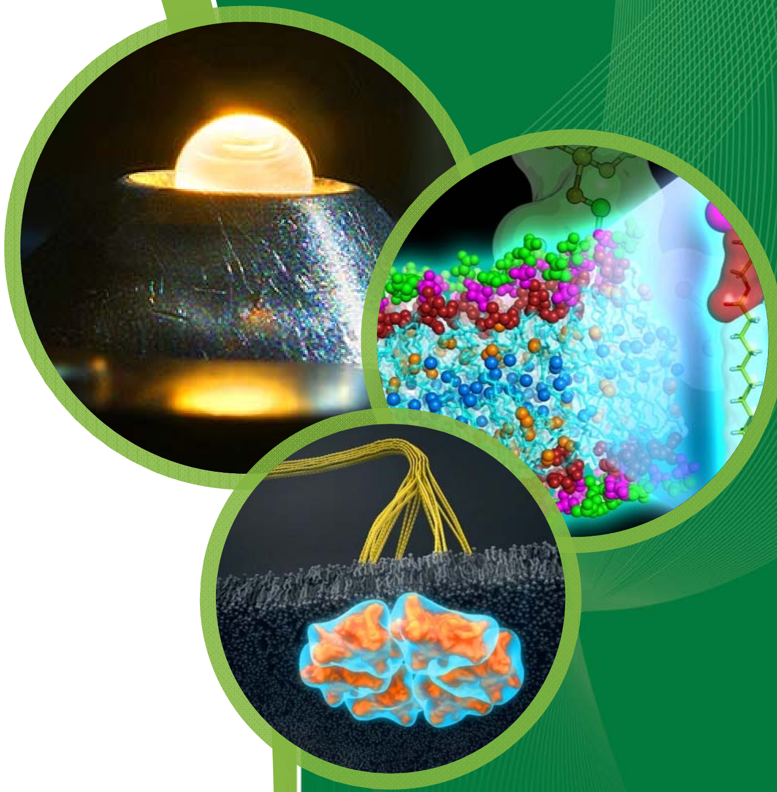
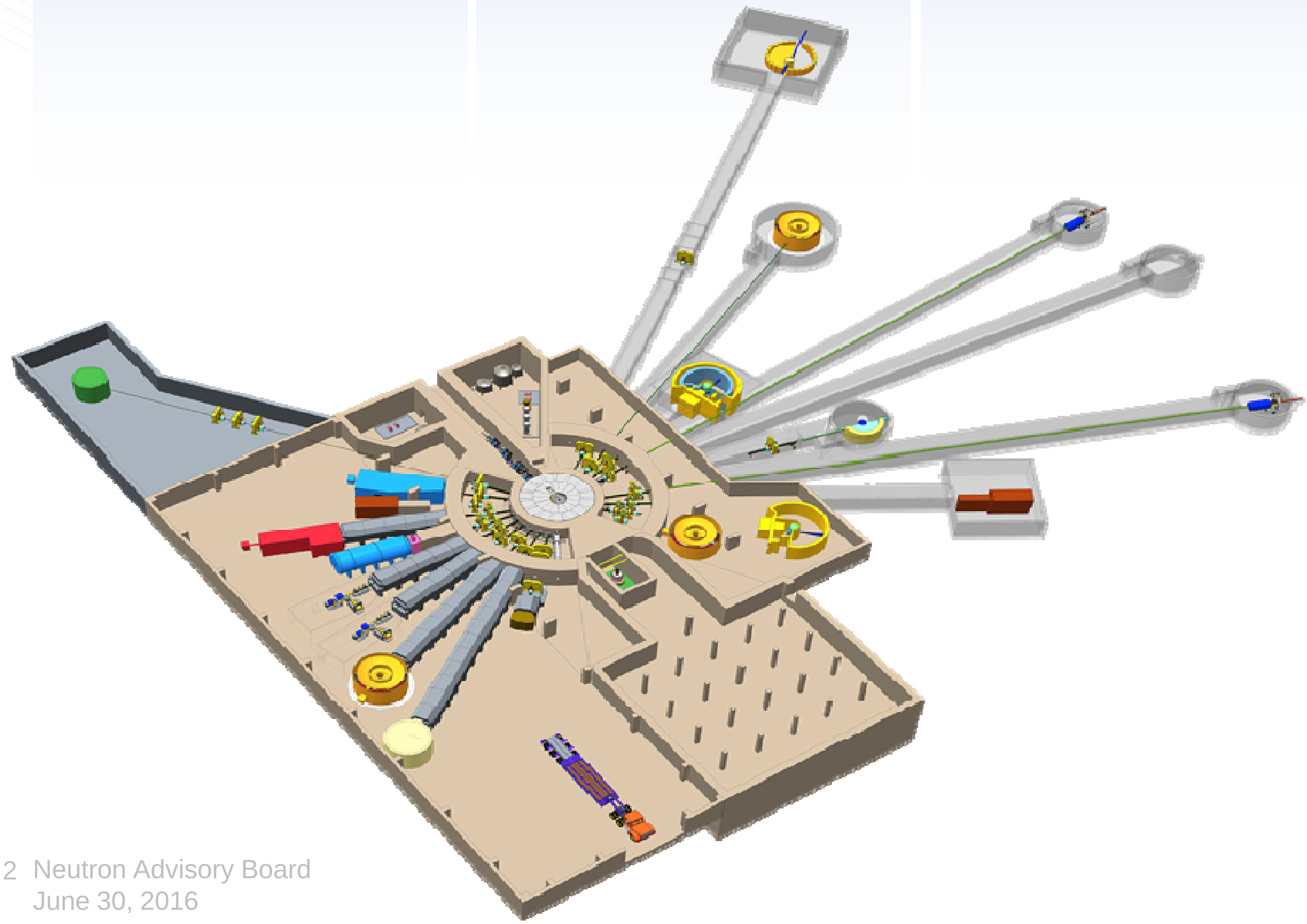
Clinch River Cabin
Oak Ridge, Tennessee



STS is a next generation source that will deliver highest peak brightness pulses of cold neutrons and ensure US leadership

Complements HFIR and FTS to ensure US leadership	Designed for complex and hierarchical materials	Highest brightness source	22 instrument end stations - 8 day one instruments

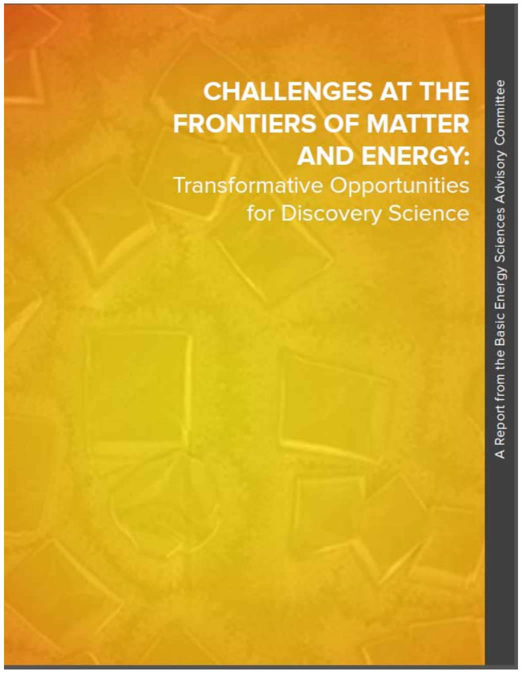


Next generation neutron source

- Compact target/moderator technology
- Integrates revolutionary advances in theory and computing on multimodal beamlines
- Spin manipulation of electrons, nuclei, and neutrons
- Advanced concepts for optics

STS provides game changing performance to meet emerging BES needs

- Mastering Hierarchical Architectures and Beyond-Equilibrium Matter
- Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder
- Harnessing Coherence in Light and Matter
- Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing
- Exploiting Transformative Advances in Imaging Capabilities across Multiple Scales



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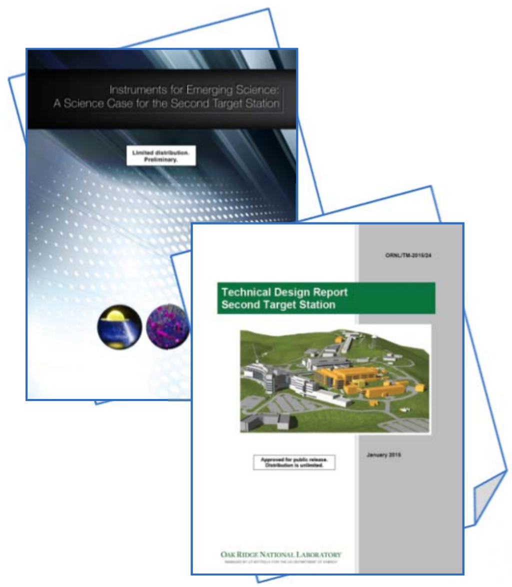
Identifying emerging scientific challenges and technical solutions to address user needs

December 2013–March 2015	October 2014	October 2015
Workshops with scientific community representatives to identify Grand Challenges for Neutrons	ORNL staff and external experts construct draft Technical Design Report (TDR) and science case	STS user meeting organized jointly with SNS-HFIR User Group develops instrument needs and selects 12 instruments to be considered for full design



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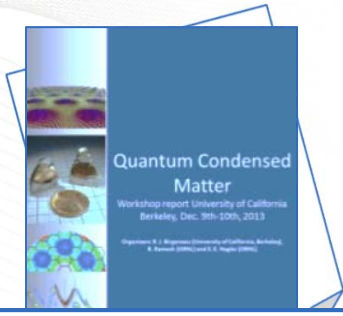
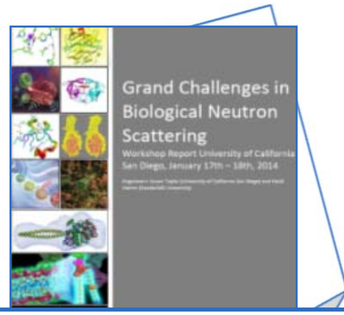
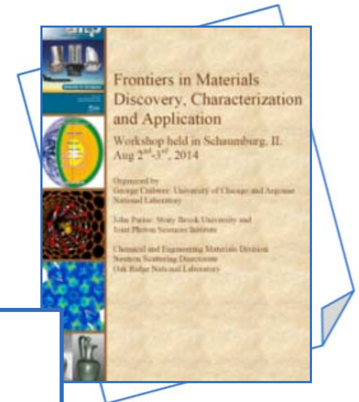
Grand challenge workshops defined future neutron user community needs

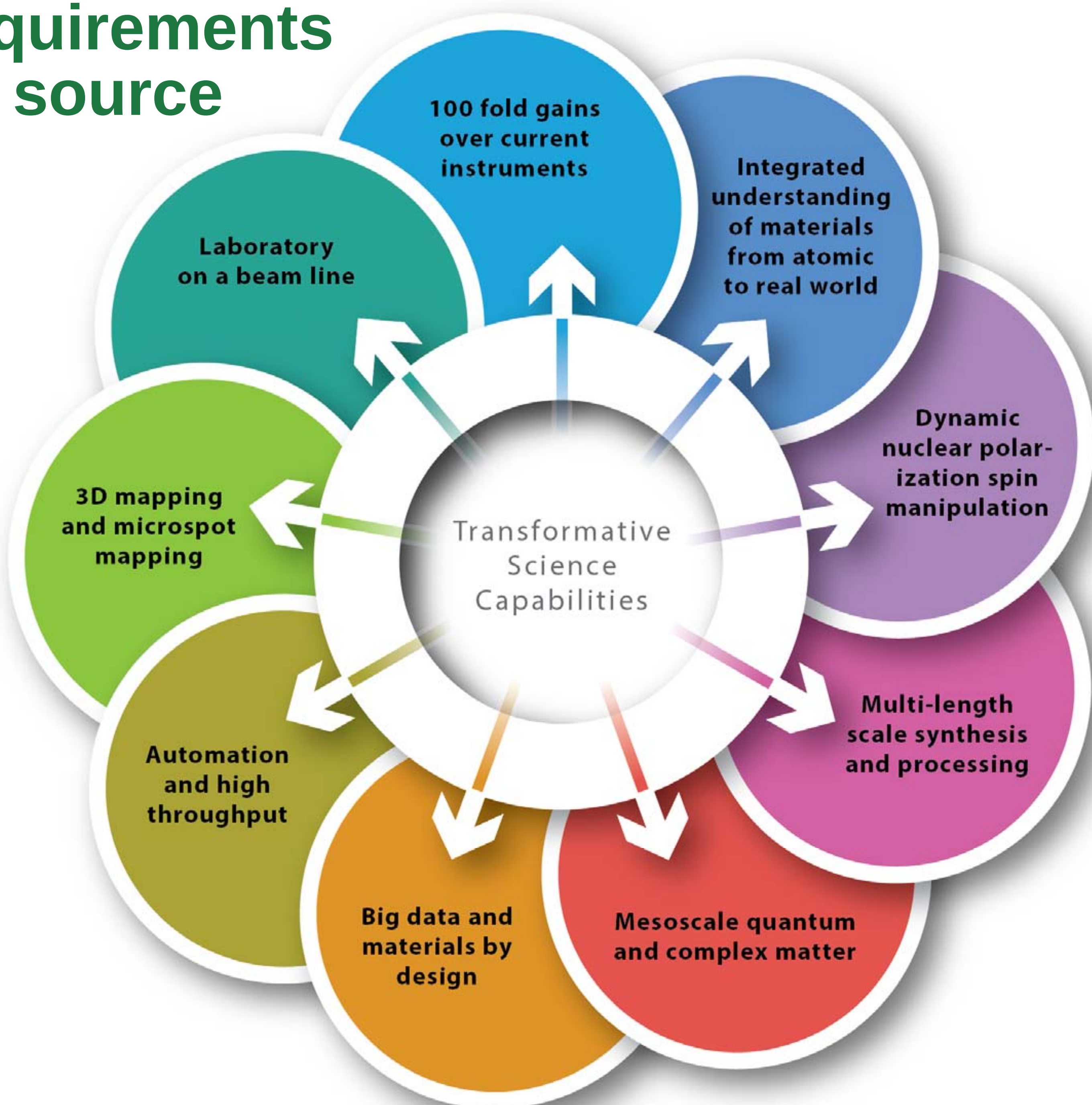






- Access to phenomena at new extremes of pressure: Dynamics at 100 GPa
- Accessing active materials and stimuli
- Applied materials and systems: Engineering
- Beyond ideal materials/ systems: Chemical synthesis, batteries, catalysis, environmental management
- Exploring coherence in matter: Full polarization and focused beams
- Future quantum devices and materials: Dynamics of heterostructures and nanomaterials
- Hierarchical architectures and beyond-equilibrium matter
- Neutron scattering at the frontier of high magnetic fields (40 T and beyond)
- Quantum materials out of equilibrium: Pump probe capabilities
- Understanding complex biosystems and the crucial role of hydrogen

Meeting requirements needs new source



Innovative STS design enables new science to meet BES needs

STS capabilities

High peak neutron brightness
- High-throughput – in situ sample synthesis
- Out-of-equilibrium behavior phenomena
- Kinetics: Time-dependent phenomena
- Small samples – microspot scanning
- Parametric studies

Cold neutrons
- Nano- to mesoscale phenomena
- Slow dynamics
- Neutron spin manipulation
- Beam focusing

10 Hz operation
- Simultaneous access to wide range of length/time scales
- Wavelength dispersive methods
- Extreme sample environments (limited angular access)
- Limits heat deposition in compact target

High-performance computing
- Real-time manipulation/visualization of massive data sets
- Combine and interpret multi-technique data
- Linking experimental data and theory
- Unified reconstruction of imaging and scattering data

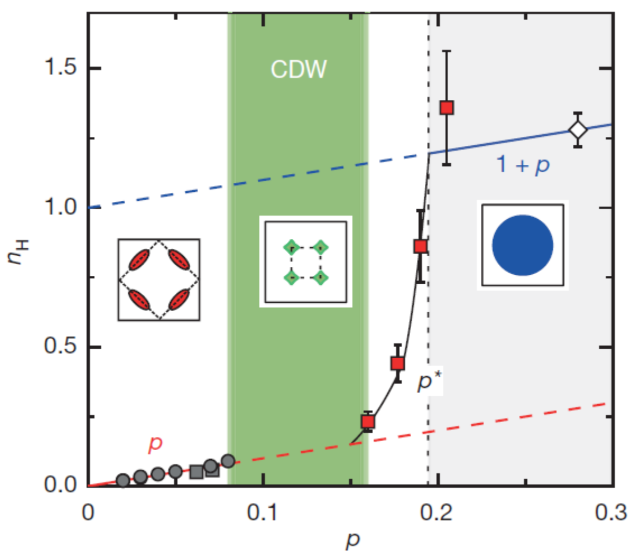
Innovative instrument concepts
- Orders of magnitude performance gains
- Integrated polarized neutron capabilities
- Manipulate sample nuclei and electron spin in situ
- Multimodal and flexible reconfiguration
- Beam line as a lab

ZEEMANS

Exploring new frontiers in quantum materials

Why STS?

Matching high brightness cold neutrons with steady and pulsed field strengths now available only at a few magnet labs worldwide will bring the unrivaled capabilities of neutrons in probing magnetism and superconductivity to a host of new quantum materials and phenomena



Nature of the quantum critical point in high-T_c superconductors

Neutron scattering uniquely measures the low energy fluctuation in the field induced normal state, identifying the underlying QCP

Opportunities

Quantum matter at extremely high fields (40 T)

Field alignment of materials; new methods for processing and synthesis

Access to and control of exotic phases and transitions

Strong perturbation of electronic orbits and magnetic states

Multipurpose beamline integrated with a high-field magnet: SANS, imaging, diffraction, inelastic scattering in a single instrument

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HERTZ

Elucidating origins of quantum coherence in materials

Why STS?

The advent of routine full polarization analysis at STS and focused neutron beams will provide game-changing capabilities for exploring entangled quantum states

Expose relativistic fermions with 4D polarized tomography

Weyl semimetal Mn_3Sn shows record anomalous Hall effect at room temperature

Polarization will access Weyl scattering

Opportunities

- Routinely measure full dynamical spin tensor $S_{\alpha\beta}(Q,\omega)$ in 4D space, giving complete information for first time
- Provide critical data to validate theory and modeling
- Unique insight into electronic states
- Spin-orbital phases: Topological materials
- Highly entangled quantum spin liquids
- Separate sensitive magnetic signals and continua
- Immediate access to materials when discovered

MENUS

Probing next-generation materials for real-world applications

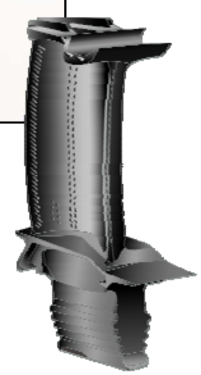
Why STS?

Neutrons are highly penetrating and have excellent properties for understanding the performance of materials in operation

Transformative gains in simultaneous imaging and mapping at STS provide critical capabilities for understanding advanced materials for manufacturing, transportation, and nuclear energy

Improving reliability of critical engineering components

In situ combined diffraction, contrast tomography with high-resolution reciprocal space mapping, and SANS nanoscale cluster characterization to understand creep fatigue



Opportunities

- Simultaneous multiscale measurements
- Advancing manufacturing of (e.g.) critical aviation structures
- Reproducing real operating conditions
- Exploiting sensitivity to light elements: Corrosion, aging effects
- Validating multiscale models directly on beamline

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Transforming capabilities for studying complex and hierarchical matter

HiRes-SWANS

Why STS?

Neutrons are an indispensable probe of soft matter

STS can directly address challenges posed by the multiple length and time scales of hierarchical systems, and explore metastable and out-of-equilibrium behavior

Understanding hierarchical fluid structures

Coacervate hydrogel: Local water dynamics shows "partitioning" into slow coacervate "compartments" and faster PEG "matrix"

Opportunities

- New classes of multiscale instrumentation
- Response of mechanical deformation
- Mechanical deformation and non-equilibrium stress
- Soft/hard composite materials
- Transport in soft matter
- Polyelectrolytes
- Complex structures in solution
- Soft matter under processing
- Quantitative measurements
- Interfaces
- Polar solvents other than water

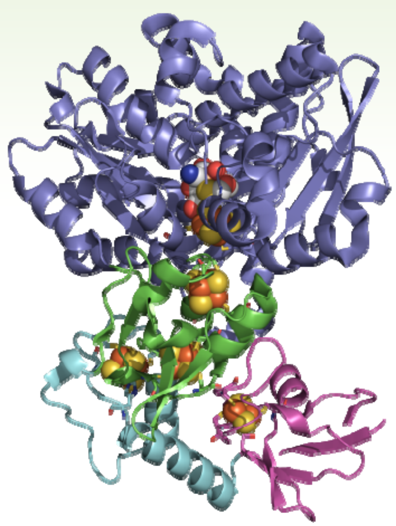
Dypol-EWALD

Elucidating the crucial role of hydrogen in biosystems

Why STS?

STS combined with deuteration will give unprecedented access to disordered proteins and membranes through structure and dynamics

Revolutionary structure determination capabilities will bring critical information on the role of hydrogen in enzymes



Multifunctional catalysts inspired by nature

Understanding the complex catalytic cycle of H^+ reduction and H_2 oxidation in hydrogenase will inspire design of novel systems and devices for H_2 production

Opportunities

- Using full structural information to design drugs
- Understand structure and dynamics of biological systems and membranes
- Study membranes and complexes in living cells
- Build predictive understanding of complex biological systems
- Understand photosynthesis and other biological processes as a basis for new biomaterials
- Understand roles of disorder and flexibility
- Determine kinetics of signaling events

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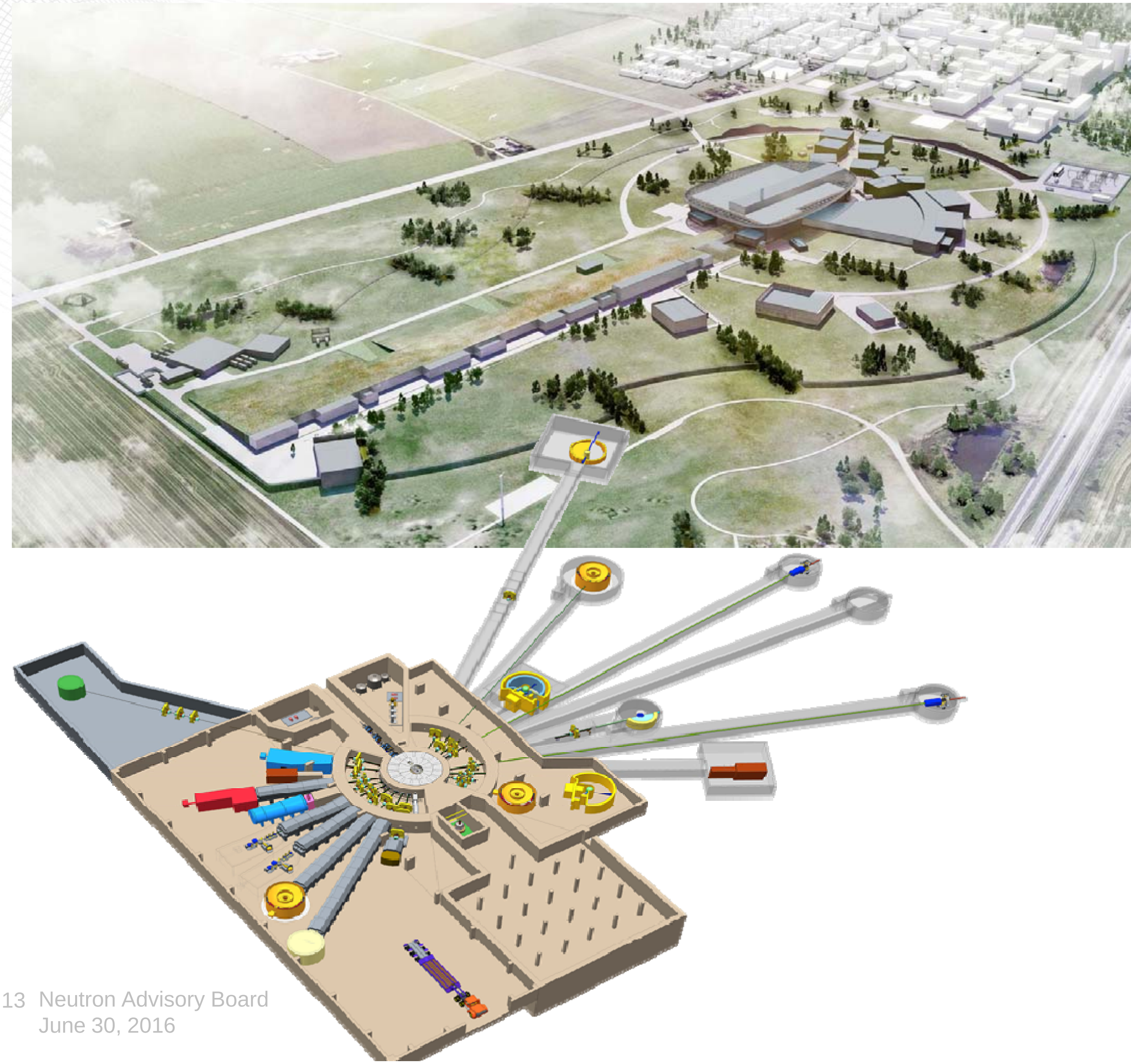
STS is needed now to ensure US leadership in science



European Spallation Source

Next generation source

- **Beam on target 2019**
- **Game changing performance in BES discovery science areas**
- **Will give Europe leadership unless STS is built**
- 5MW power - long pulse
- Integrates revolutionary advances in theory and computing on multimodal beamlines
- Spin manipulation of electrons, nuclei, and neutrons
- Advanced concepts for optics

Further actions FY17-18

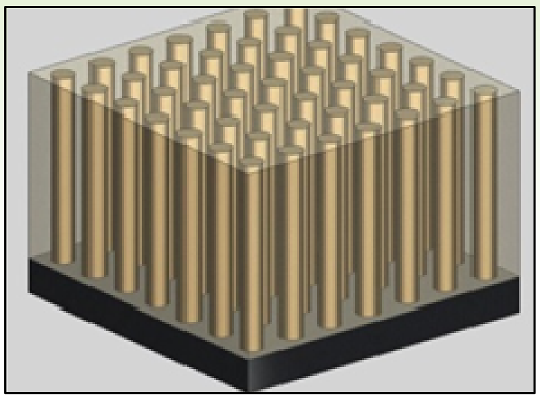
- Hold regional STS science symposia
- Out of this identify ten ground breaking experiment cases
- Work through fully including simulations of experiments on STS
- Produce ground breaking experiments document

Designing properties of interfaces and devices

Why STS?

Measure dynamics with neutrons in previously inaccessible heterostructures and nanomaterials

Access knowledge on couplings essential for design of spin- and quantum-based devices



Superconductivity with interface engineering

Measurements of dispersions of phonons and spin waves at and near interfaces in FeSe/STO composites will give vital information for boosting T_c

Opportunities

Probing the spin and lattice dynamics of interfaces and nanostructures to reveal nature and strength of couplings

Beam intensity allows studies of (e.g., artificial crystals and heterostructures)

Neutrons are ideal to measure ionic manipulation of spin and charge states (e.g., for neuromorphic devices)

Dispersion and lifetime of measured magnetic excitations reveal magnetic transport behavior

CHESS

Accessing dynamics at extreme pressure

Why STS?

Neutrons provide vital information on magnetic states and atomic environments through spectroscopy

Matching the development of large-volume diamond anvil technology and brightest beams at STS will transform our ability to study matter at pressures of 100 GPa and beyond

Correlations and topology in SmB_6

Spin dynamics and pressure give critical insight into correlations in a topological insulator

Opportunities

- High-intensity beams for spin, phonon, and vibrational dynamics at 100 GPa
- Pressures strong enough to break and rearrange covalent bonds
- Exotic new quantum phases and transitions
- Completely new materials and structures
- Quantum effects in hydrogenous systems and new superconductors (e.g., H_2S)
- Visualization of essential dynamics stabilizing phases

Understanding out-of-equilibrium states and switching

CHESS

Why STS?

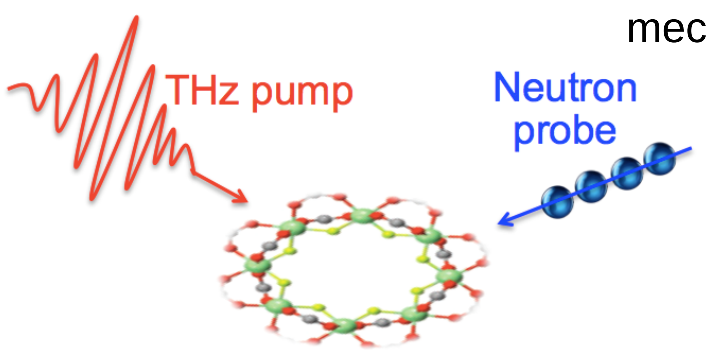
Pulsed fields, THz radiation, and optical switching afford methods of transitioning between states

Harnessing STS brightness and pulse structure enables monitoring the evolution of states out of equilibrium (e.g., in long-lived molecular magnets)

Non-equilibrium quantum dynamics

In molecular magnets, neutrons give spatial and temporal information on their wave functions

Observing the evolution of these states out of equilibrium will transform understanding of the relaxational mechanisms



Opportunities

Spintronics

Magnon transport in antiferromagnets

Skyrmions in driven conditions

Quantum and molecular magnets

THz pumping of populations

Transport and decoherence in quantum states

Optical switching

Light-activated magnetic switching

Addressing complex energy and environmental systems

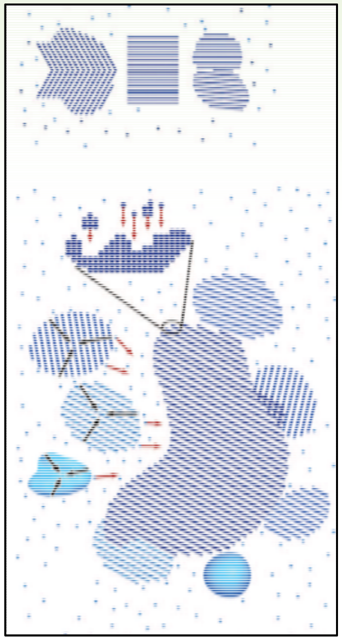
Why STS?

Neutrons are essential to look at light elements at interfaces, reactions, and systems under realistic conditions

Powerful multi-modal capabilities of STS promise transformative gains in understanding systems relevant to chemical synthesis, batteries, catalysis, and environmental management

Environmental management of legacy nuclear wastes

Development and validation of predictive models of nucleation, growth, aggregation, and dissolution of solids is critical for accelerating the design of novel removal and processing strategies



Opportunities

Chemical synthesis and kinetics for light elements (H, Li, C, H_2O/D_2O)

Unique insights from transformative neutron spectroscopy

Combining crystallography and dynamics into powerful analytical technique

Composite and porous materials, element transport, and reactivity can be followed

Electrochemistry and chemistry at interfaces (e.g., using ^{6}Li, ^{7}Li labeling)

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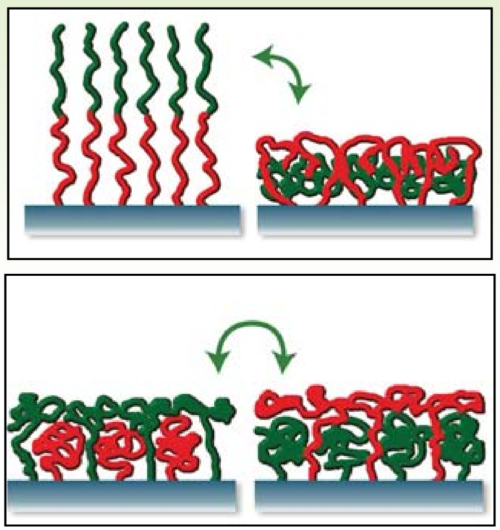
QIKR

Probing active materials and stimuli

Why STS?

STS neutrons will provide the spatially and temporally resolved maps under stimuli needed to quantitatively predict time-dependent material properties



Kinetics of stimuli-responsive smart coatings

Understand kinetics/ thermodynamics of novel responsive materials, such as selective response of polymer brushes to changes in the local microenvironment

Opportunities

- Simultaneous data collection over broad Q range; asynchronous sample-environment forcing
- Unprecedented peak cold neutron flux: Window into transient, time-dependent, and non-equilibrium processes
- Fast adsorption and desorption processes (aerosols on water, surface response to mechanical shocks)
- Fast reactions at surfaces (liquid/solid interface under shear, structure formation at battery electrodes)
- Biological processes: Initial interactions of proteins with cell membranes, biochemistry at liquid/liquid interfaces
- Polymer diffusion, gas adsorption, chemical activation in situ

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