Panel on Neutron Scattering User Facilities

Presented to:
Basic Energy Sciences Advisory Board

Upgrades to the Spallation Neutron Source (SNS)

Paul Langan
Associate Laboratory Director for Neutron Sciences
Oak Ridge National Laboratory

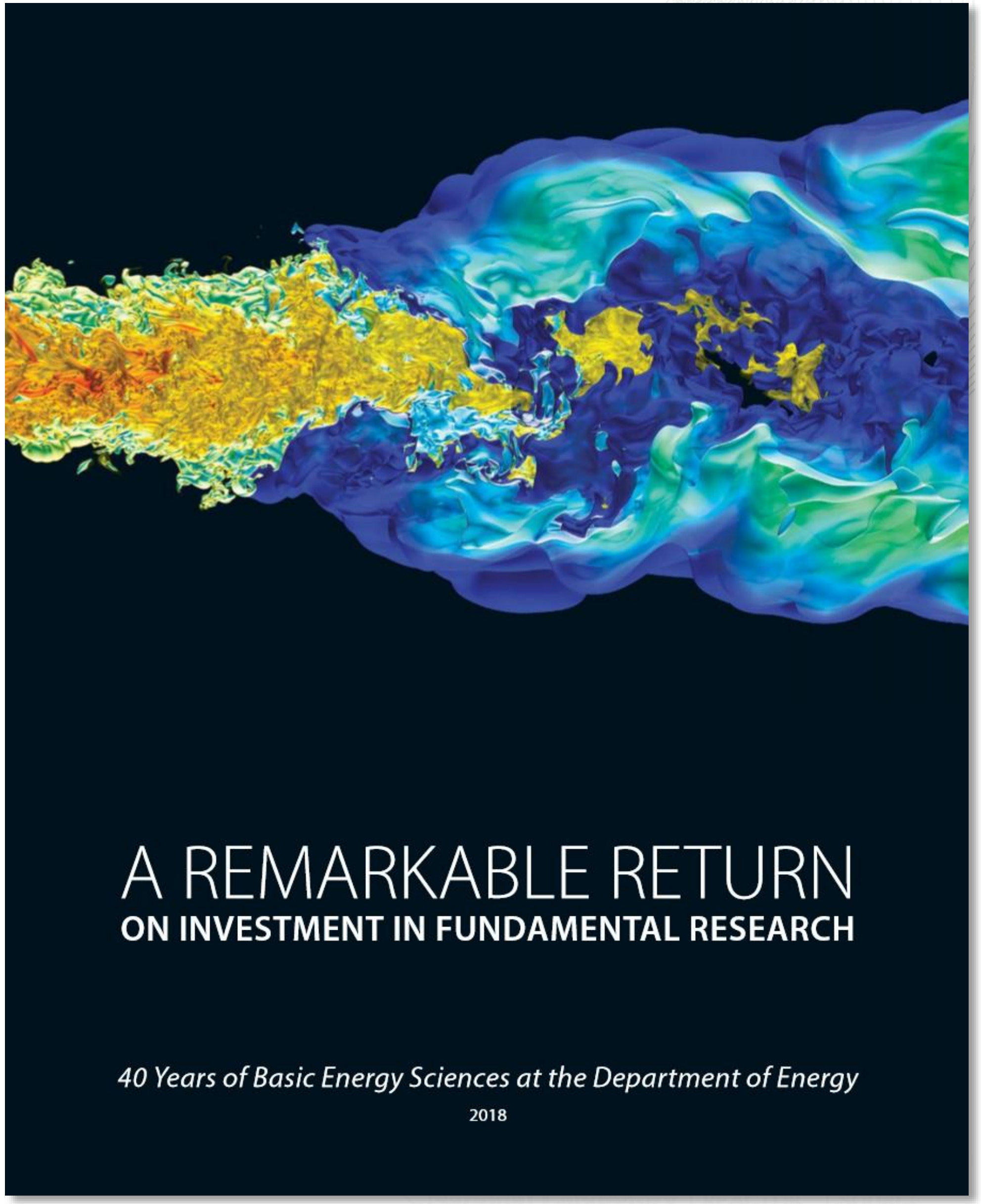
Neutron source developments in Europe and Asia

Dimitri Argyriou
Chief Research Officer
Ames National Laboratory

Addressing science priorities with SNS upgrades

Collin Broholm
Gerhard H. Dieke Professor of Physics and Astronomy
Johns Hopkins University

July 12, 2018
Bethesda



BES pioneered fission and spallation neutron sources and now operates the world's highest flux facilities

High Flux Isotope Reactor (HFIR)

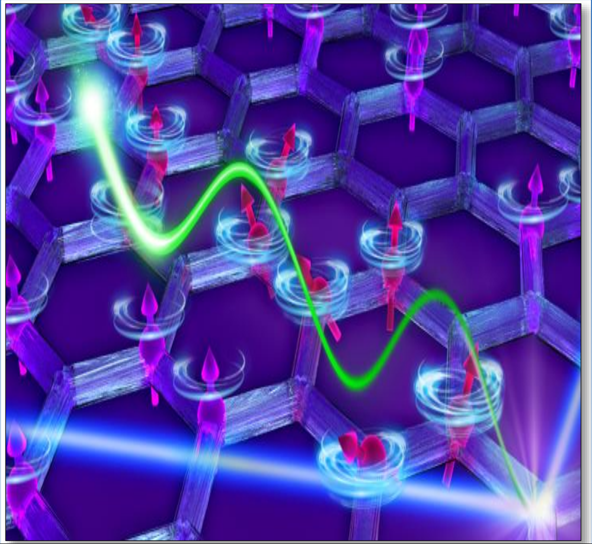
World's highest continuous neutron flux

Spallation Neutron Source (SNS)

World's highest peak neutron brightness

DOE's Oak Ridge National Laboratory is the cradle of neutron scattering.
Today, SNS and HFIR form a world-leading center for neutron scattering studies of materials.

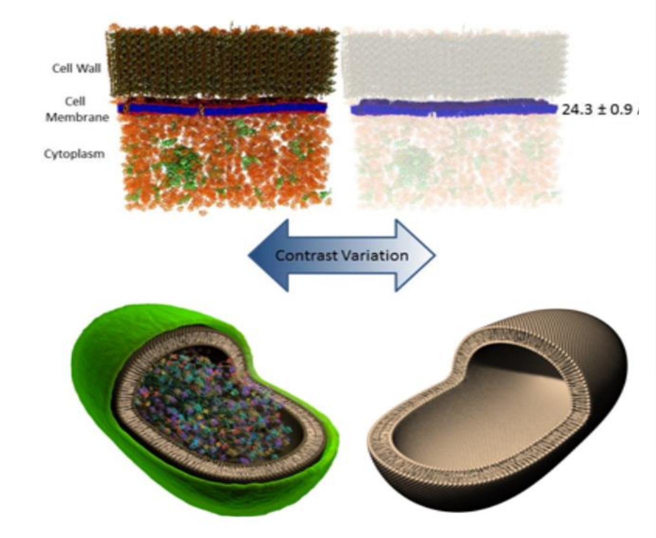
SNS & HFIR enable progress in forefront fields of research



Neutrons reveal Majorana fermions in a Kitaev quantum spin liquid

(α-$RuCl_3$ honey-comb lattice)

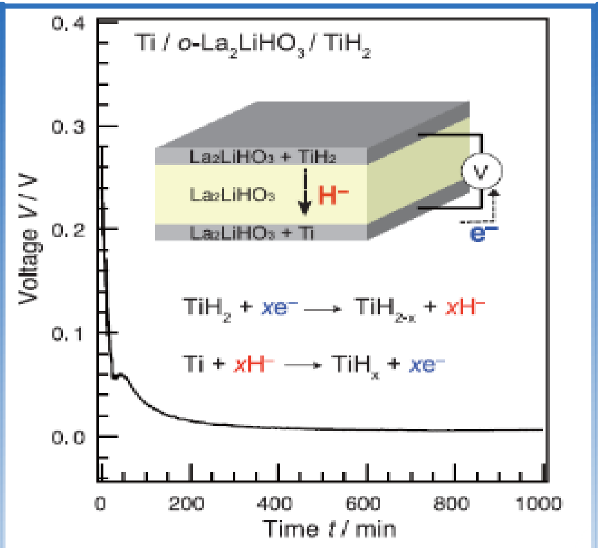
Banerjee et al., *Science* 2017



Neutrons expose lipid nanodomains in a living bacterium

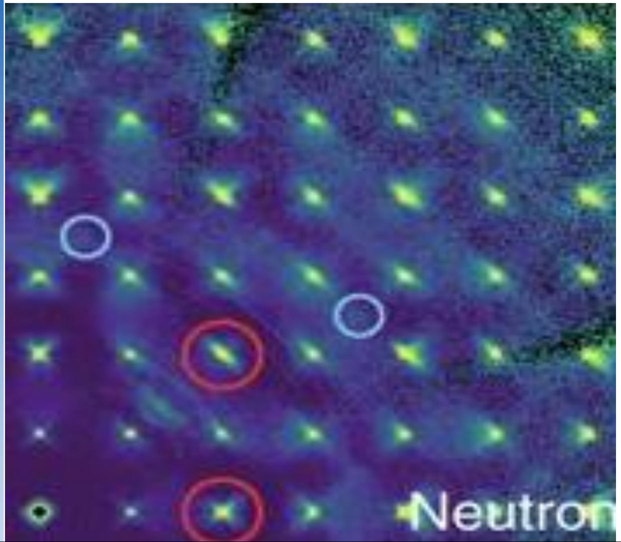
(Bacillus *subtilis*)

Nickels et al., *PLoS Biology* 2017



Neutrons validate novel proton conducting solid state battery materials

Kobayashi et al., *Science* 2016

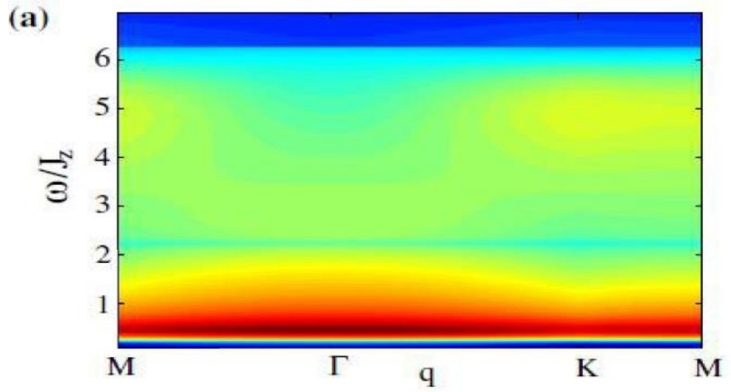


Neutrons relate ultrahigh piezoelectricity and multiscale structure in relaxor ferroelectrics

Krogstad et al., *Nature Mat.* 2018

Emerging science requires enhanced neutron scattering

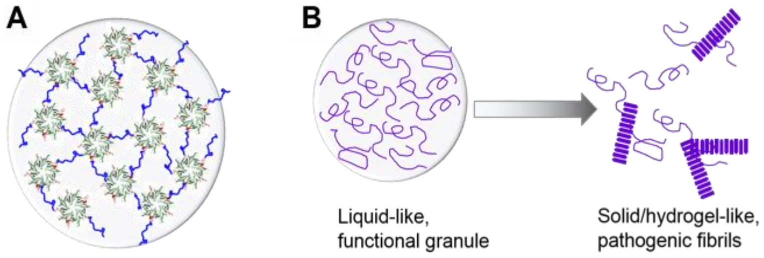
What exotic particles exist in quantum spin liquids?



More long-wavelength neutrons at the STS will provide access to lower energy (μeV) excitations and slower dynamic time-scales (μs) with high resolution

e.g. probing visons in Kitaev quantum spin liquids

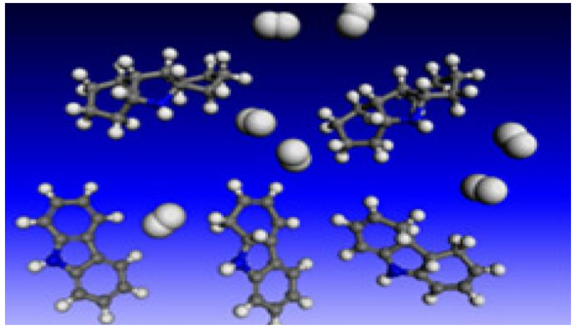
How do complexes dynamically assemble within living cells?



Beams of pulsed neutrons with **higher peak brightness** at the STS will provide access to single-pulse experiments, microsecond dynamics, and 100 millisecond time-resolutions

e.g. *in vivo* dynamic self-assembly of membrane-less organelles linked to neurodegenerative disease

What are the mechanisms of catalysis in liquids and at interfaces?



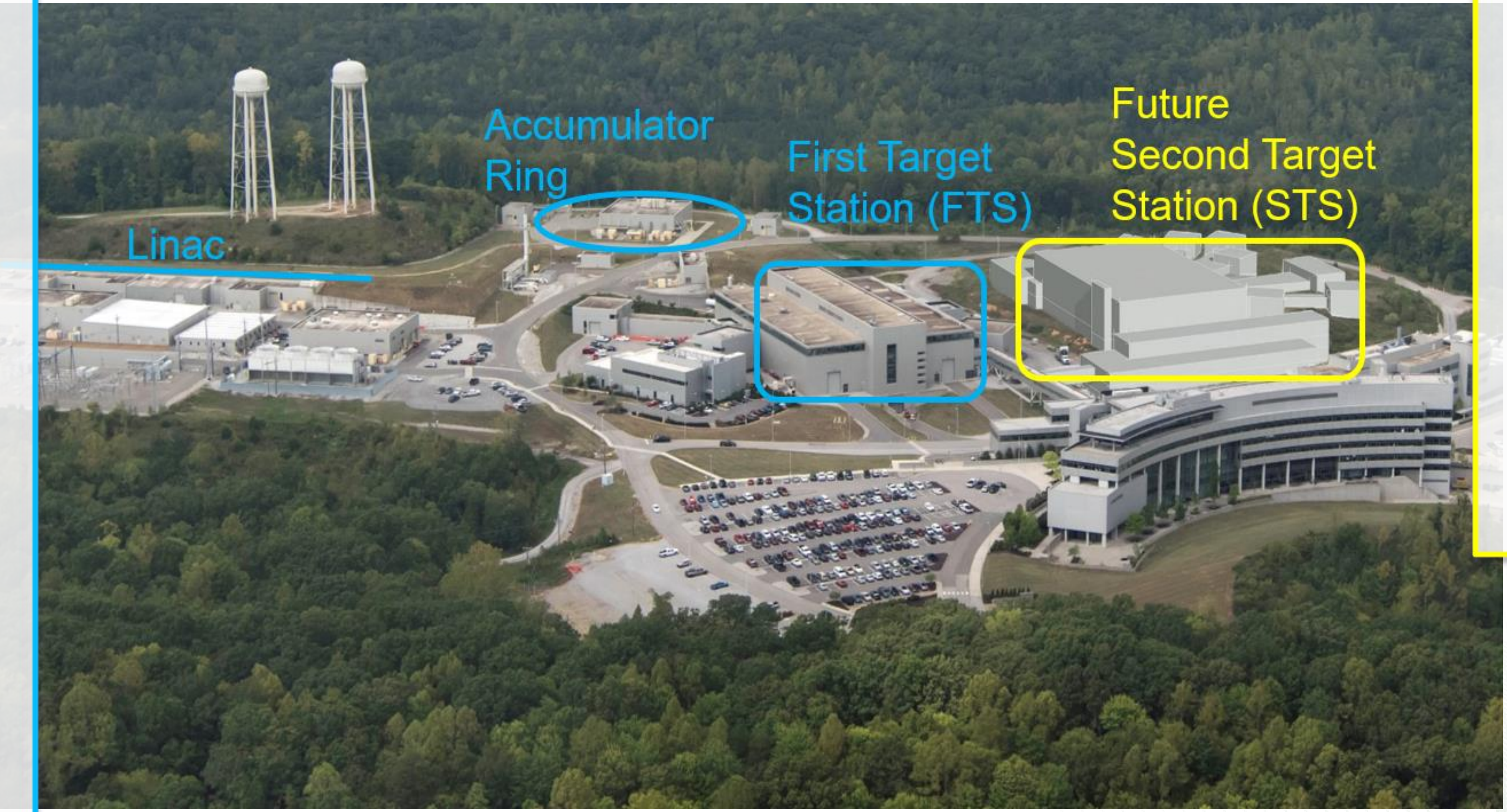
The **broad wavelength range** between short pulses of neutrons at the STS will allow simultaneous access to larger length and time scales

e.g. *in operando* catalytic reactions such as dehydrogenation of liquid organic carriers

SNS upgrades to accelerate scientific and technological progress

PPU project is an upgrade to the existing accelerator structure

- Doubles accelerator power capability
- Increases FTS neutron flux and provides new science capabilities
- Provides a platform for STS

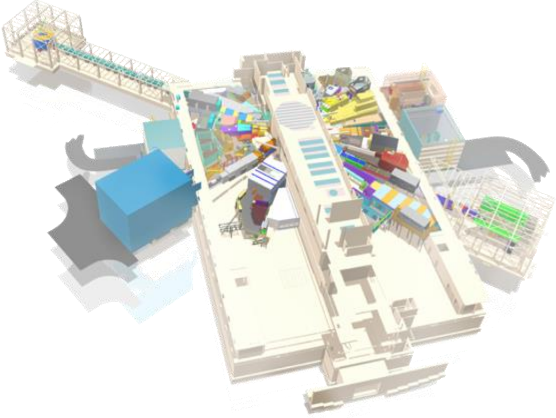


STS project is a second target station with an initial suite of beam lines

- More long-wavelength neutrons
- Higher peak brightness
- Broader wavelength range

SNS Upgrade Plans

24 instrument positions
19 instruments built

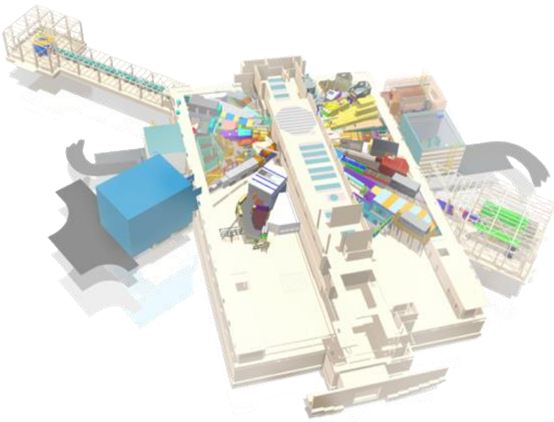


SNS First Target Station (FTS)

1.4 MW

Accelerator

Now



24 instrument positions
21 instruments built

FTS

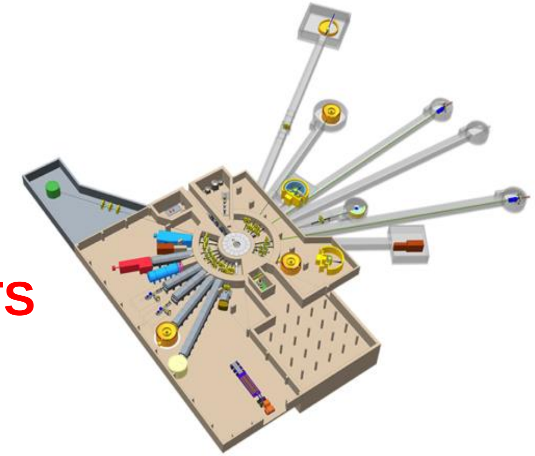
2 MW

0.8 MW

Accelerator

After PPU Upgrade

22 instrument slots, 8 initial instruments



STS

After STS Upgrade

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The scientific impact of SNS upgrades
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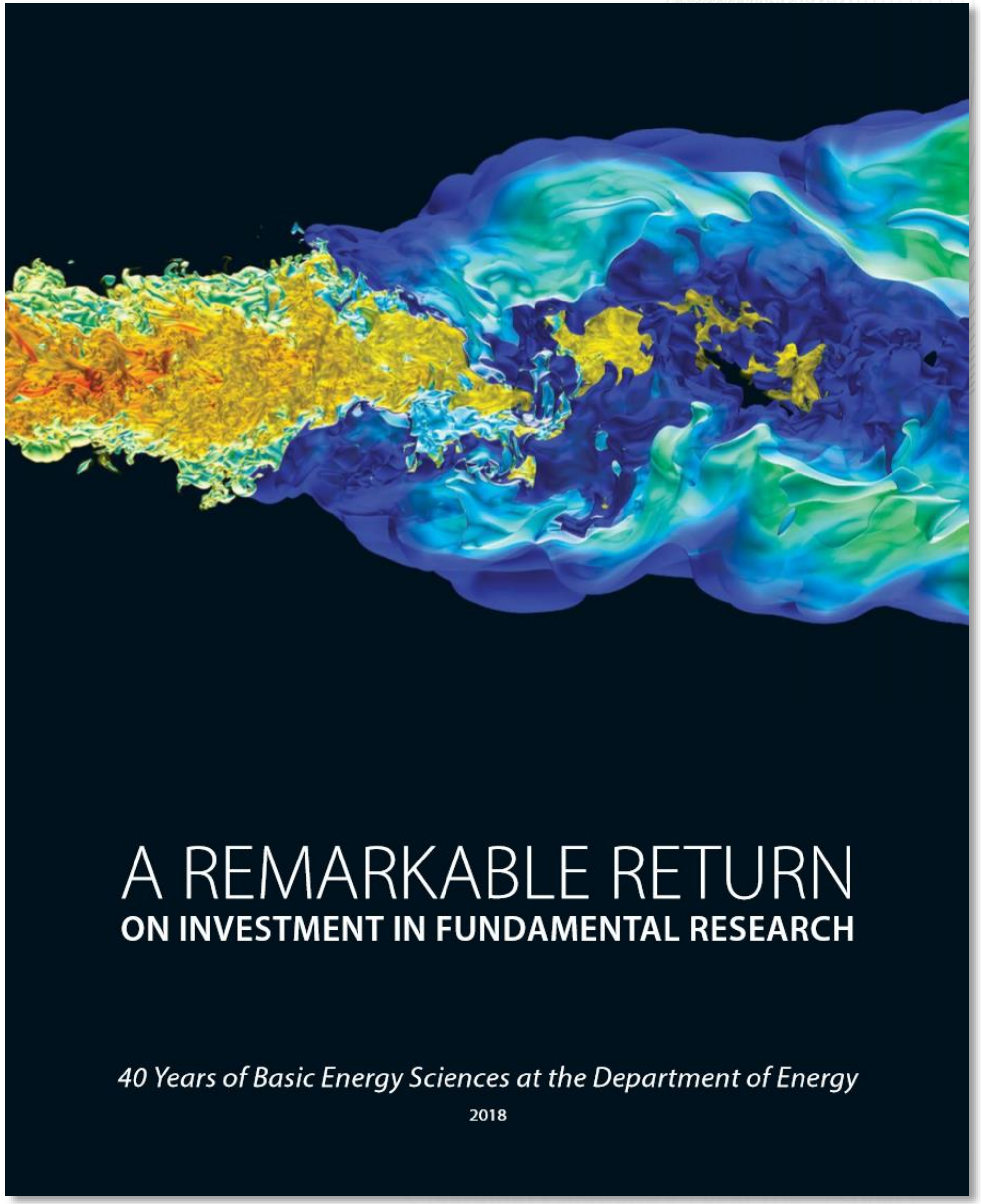
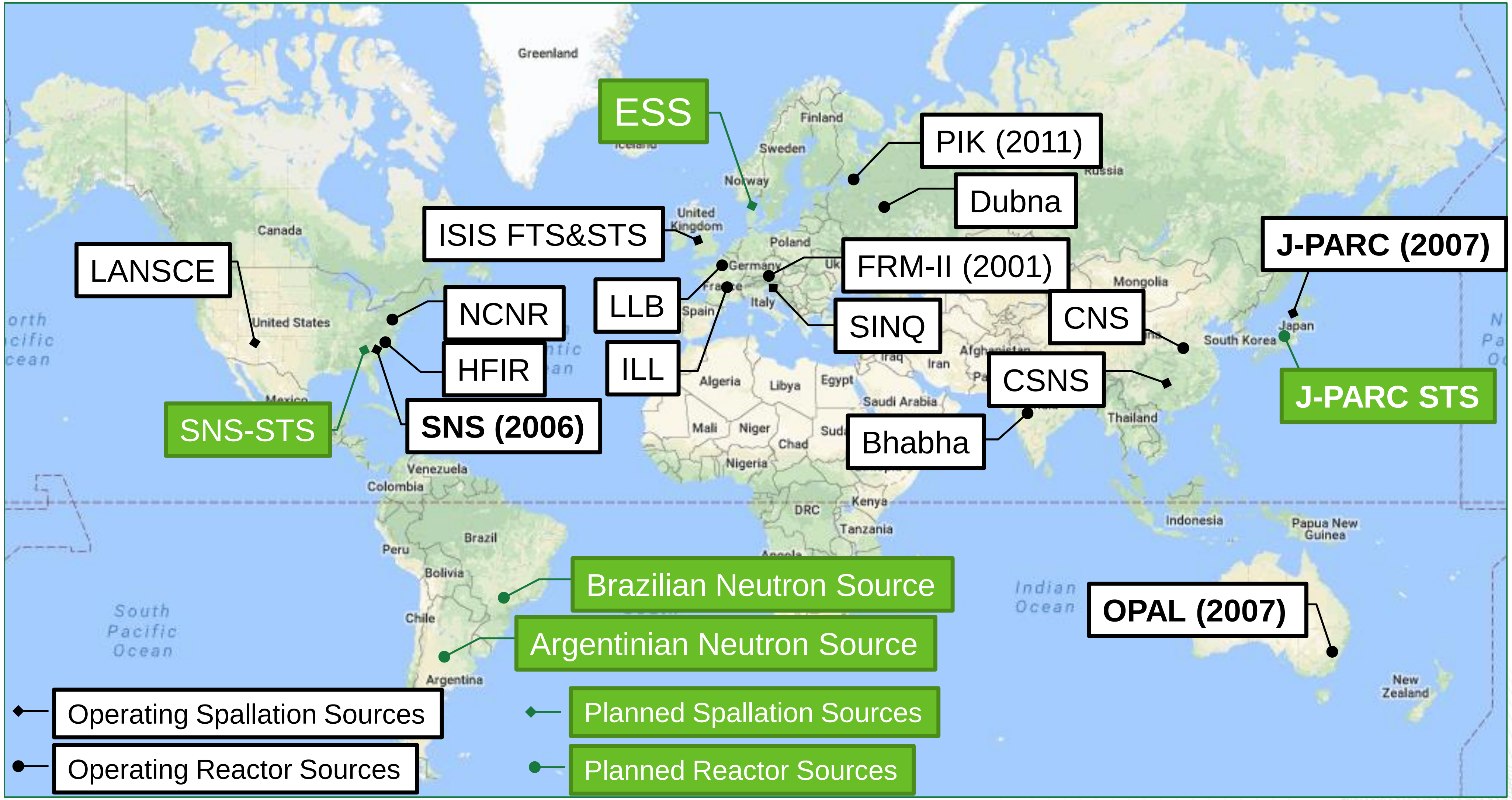


The Neutron Source Landscape is Evolving and Attracting Investment



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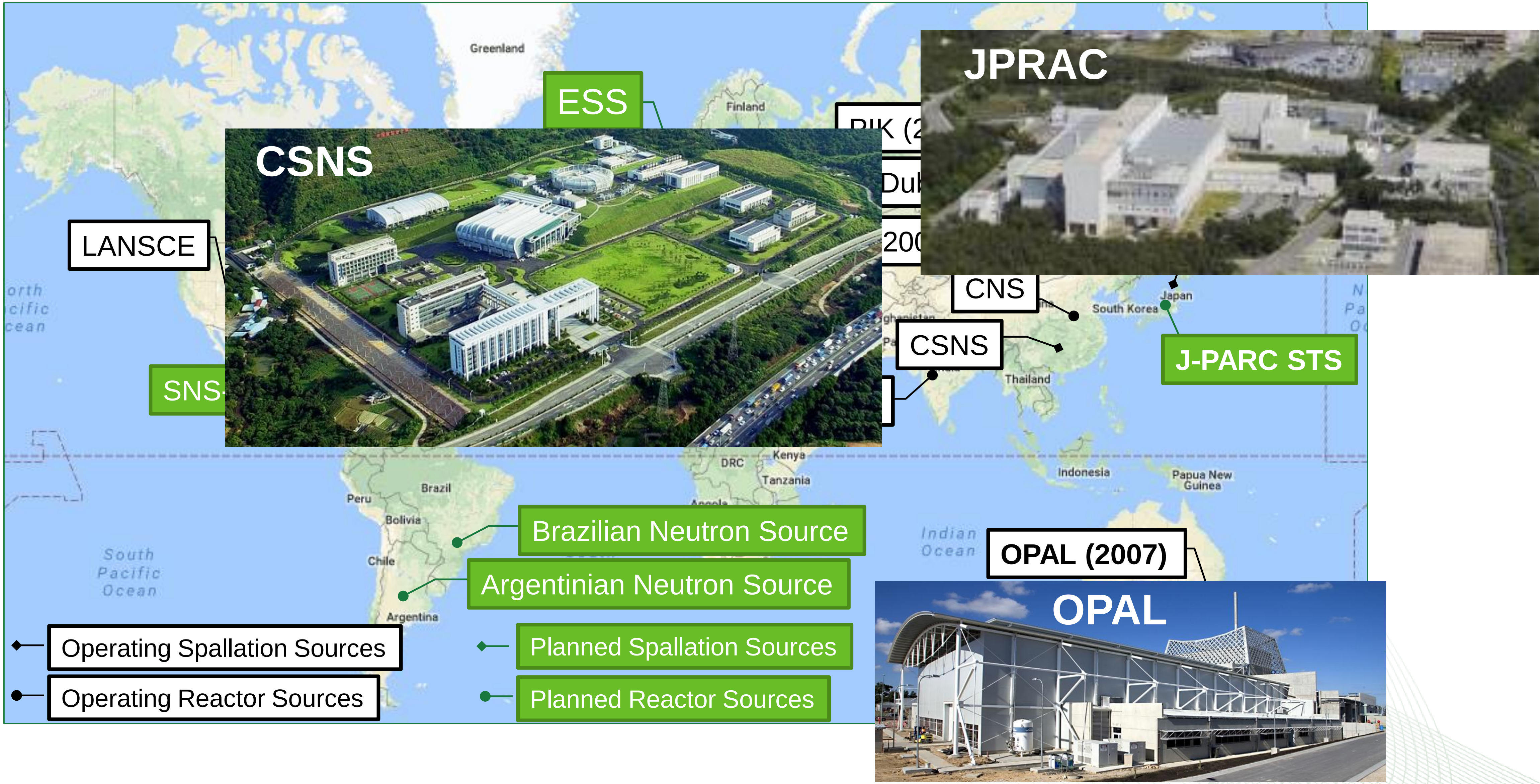

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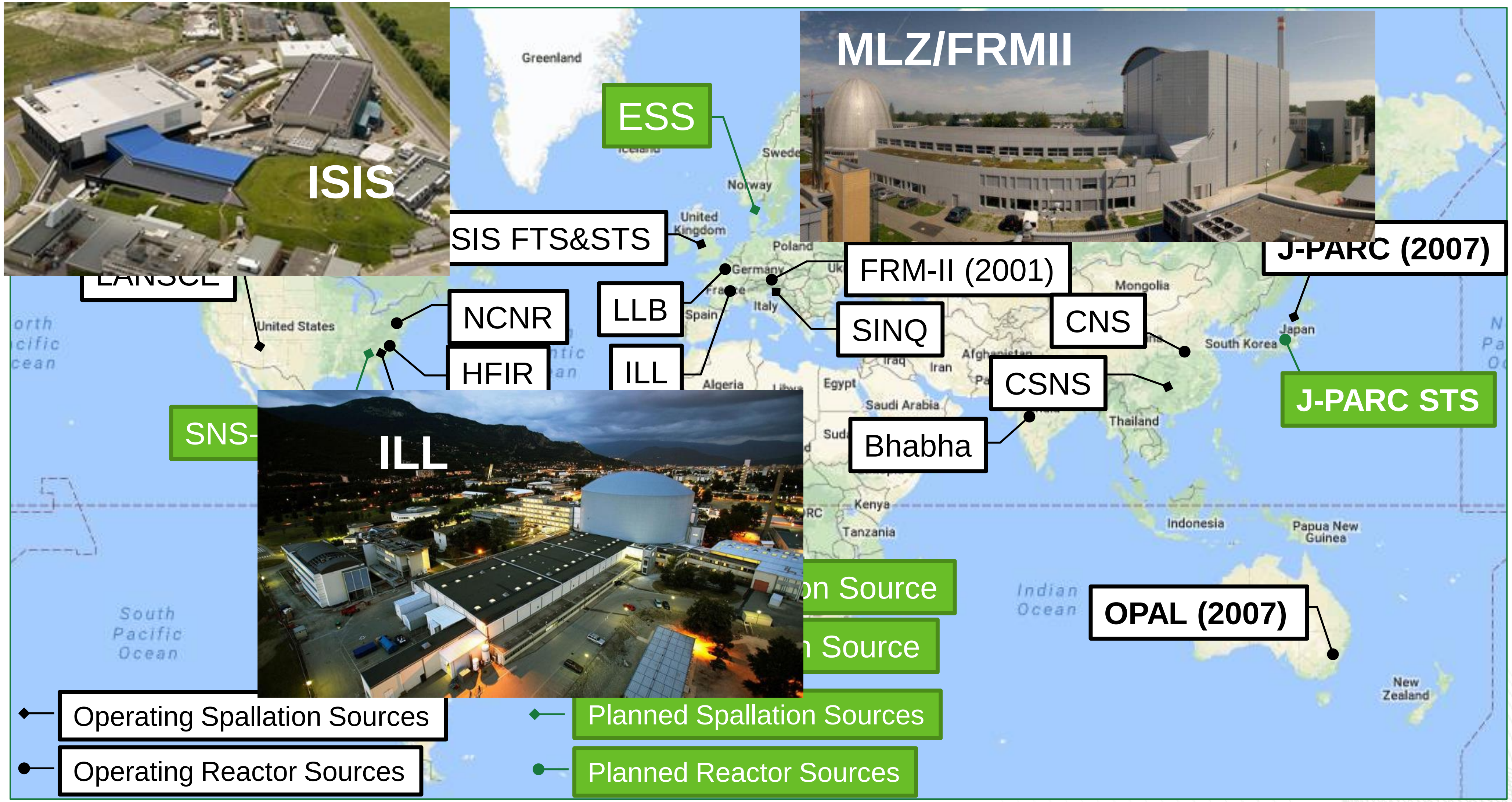
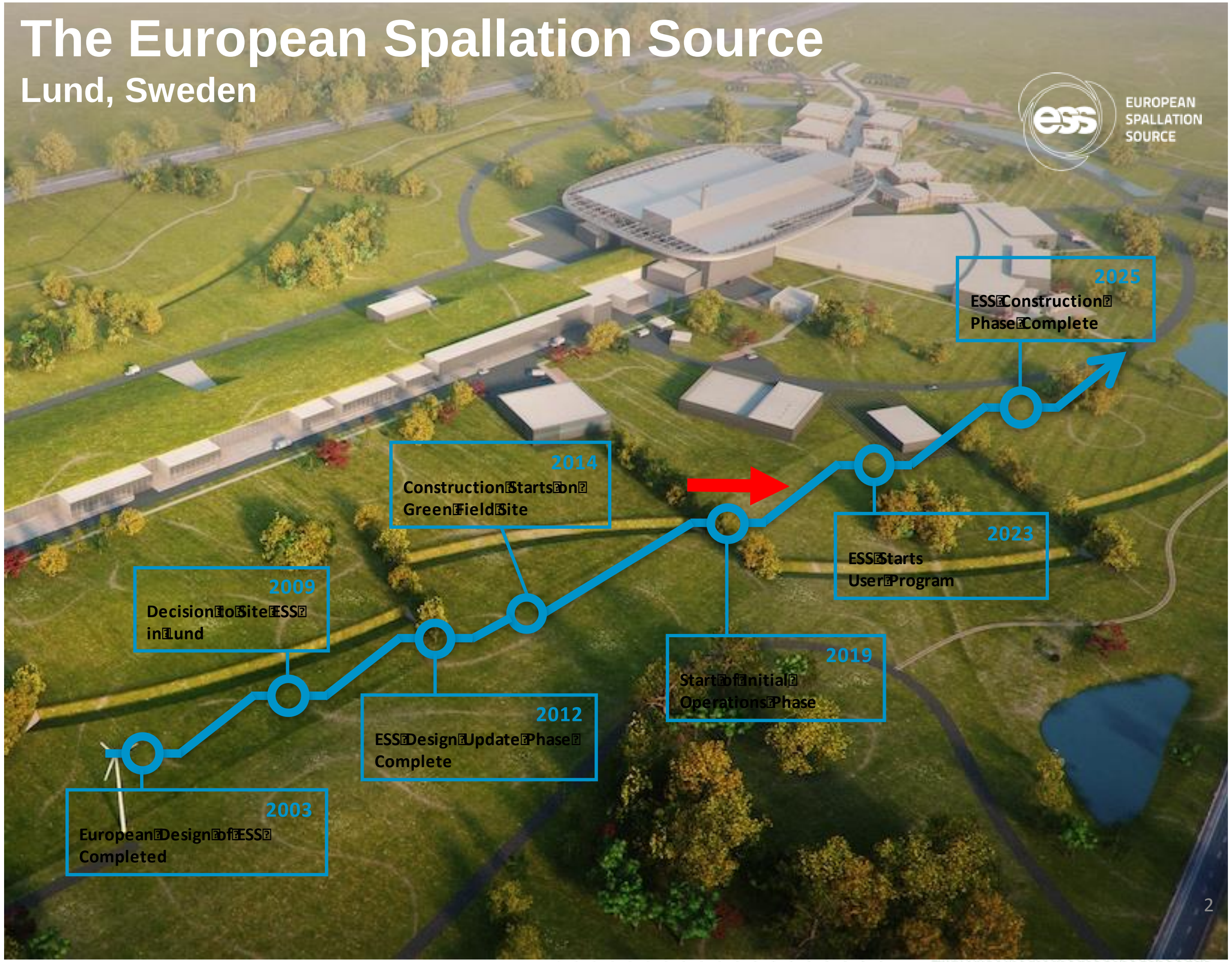


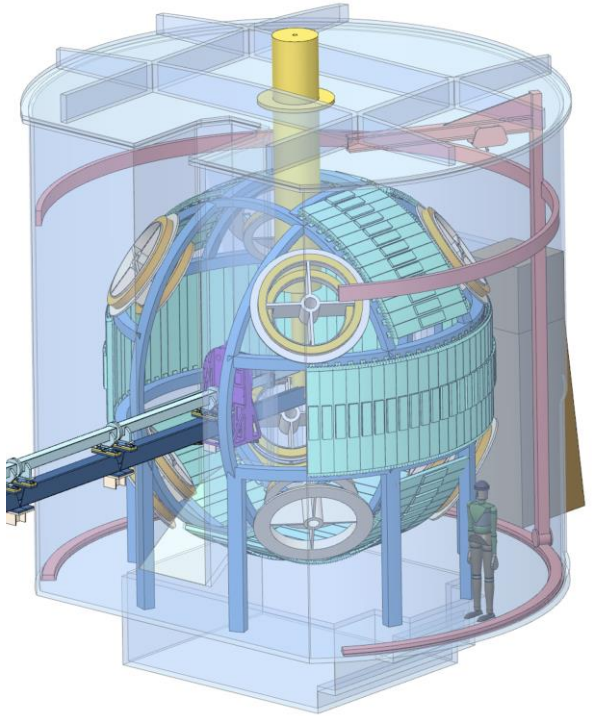
European investment in spallation sources

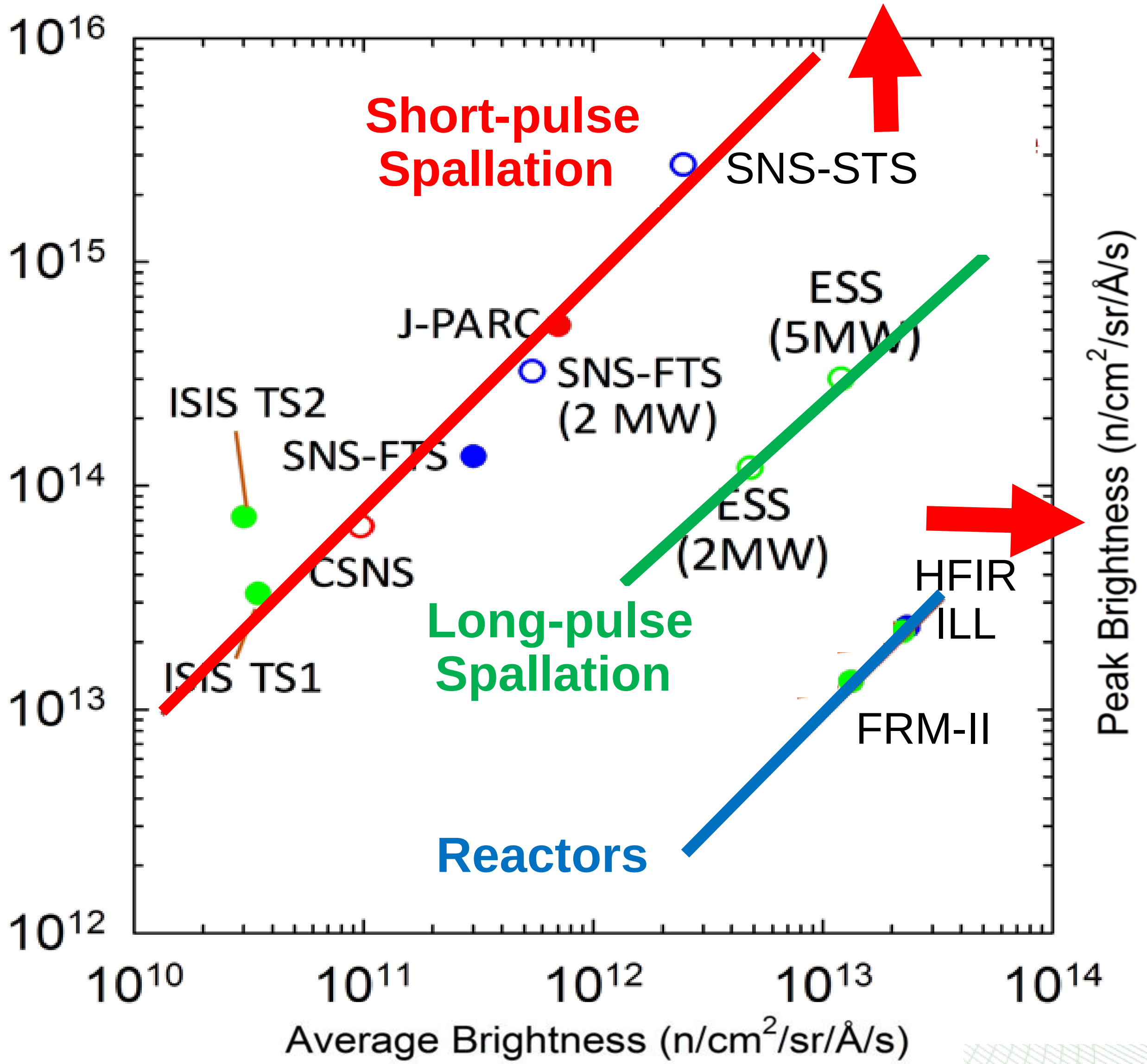
- Consortium of 16 European Countries
- $2B investment in European neutron science to serve 6000 users
- 15 Instruments in the construction budget – can host up to 35 instruments
- 5 MW proton power
- Long pulse source (~3ms@14Hz)
- Solid-W/He-cooled rotating target
- Brightness optimized (Flat) moderators
- Time-averaged flux~ ILL-reactor



As international capabilities expand, the SNS upgrades will sustain U.S. leadership in neutrons

Instrument performance gains of 100 – 1000 make STS a next generation source enabling new science



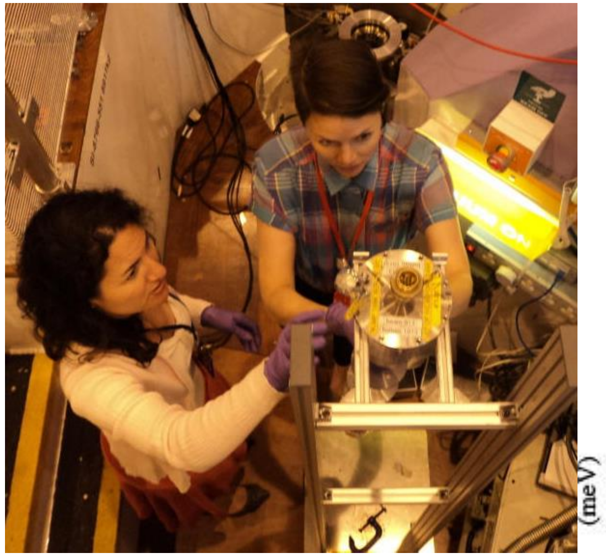


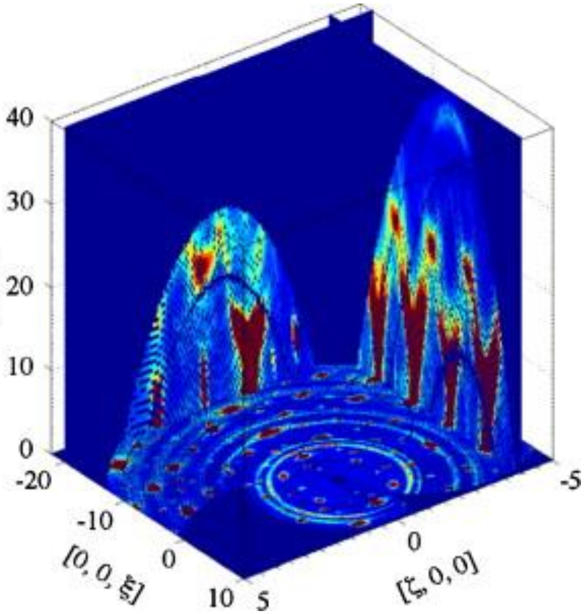
CSNS: China Spallation Neutron Source, China
J-PARC: Japan Proton Accelerator Research Complex, Japan
ESS: European Spallation Source, Sweden
ILL: Institut Laue Langevin, France
FRM-II: Forchungsreaktor Munchen II, Germany
ISIS: UK

Performance Gains via Development of Detectors, Optics and Software

- Impactful neutron science is becoming as reliant on sample environment, data analysis, and computing as on raw neutron flux

Detector Array at LET Spectrometer TS2@ISIS



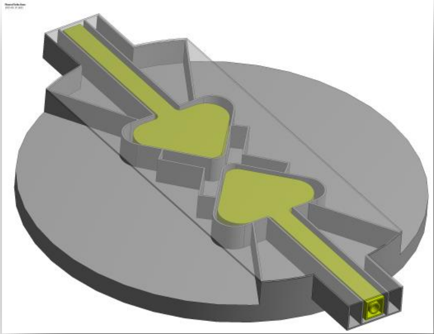


- Major gains in source performance will continue to come from innovations in moderator design, neutron optics, and detector technology in the medium term. Continual investment in these areas is **essential**.
  - Prudent to invest in new approaches for the cost effective generation of brilliant neutron beams (next generation of proton accelerators, laser driven sources etc).

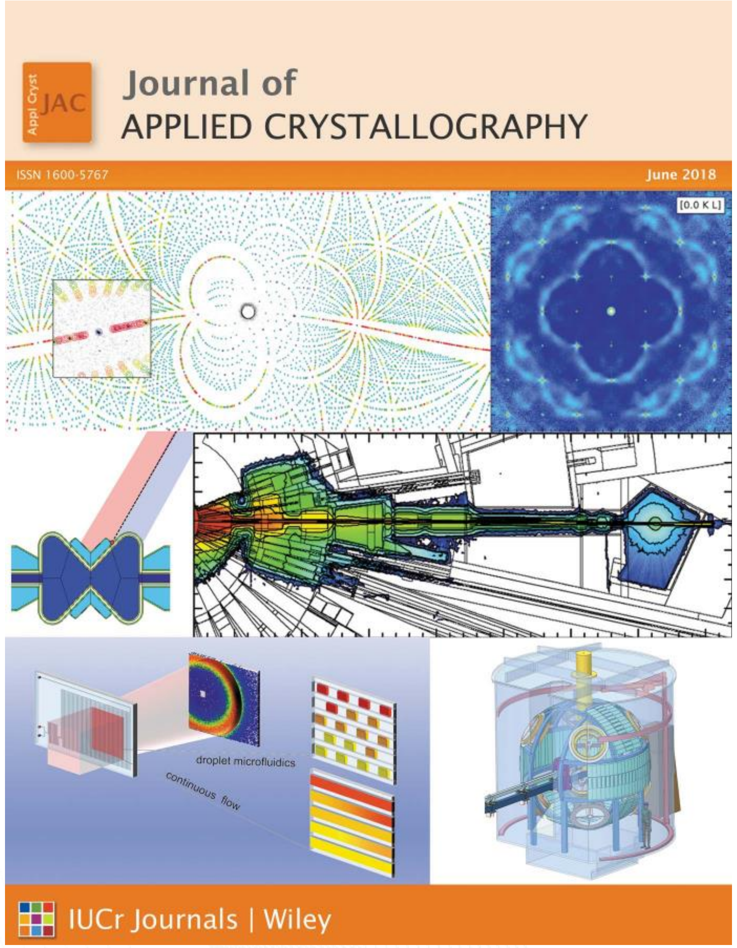
Neutron Instrumentation Evolving to Enable New Insights

- Instruments and new source designs continue to evolve to address modern science problems

- Next generation of moderators will be optimized on brilliance as opposed to flux.
  - Reduced dimensionality moderator promise relief from the 4π problem
  - Focus beams in small sample volumes



- Next generation neutron instruments focus on:
  - Deep integration with complex sample environments
  - Small sample geometries
  - High throughput/ kinetic studies
  - Increase deployment of polarized neutrons over a variety of techniques
  - Rapid mapping of $S(Q, \omega)$ at higher resolutions



Special issue on neutron instrumentation
June 2018

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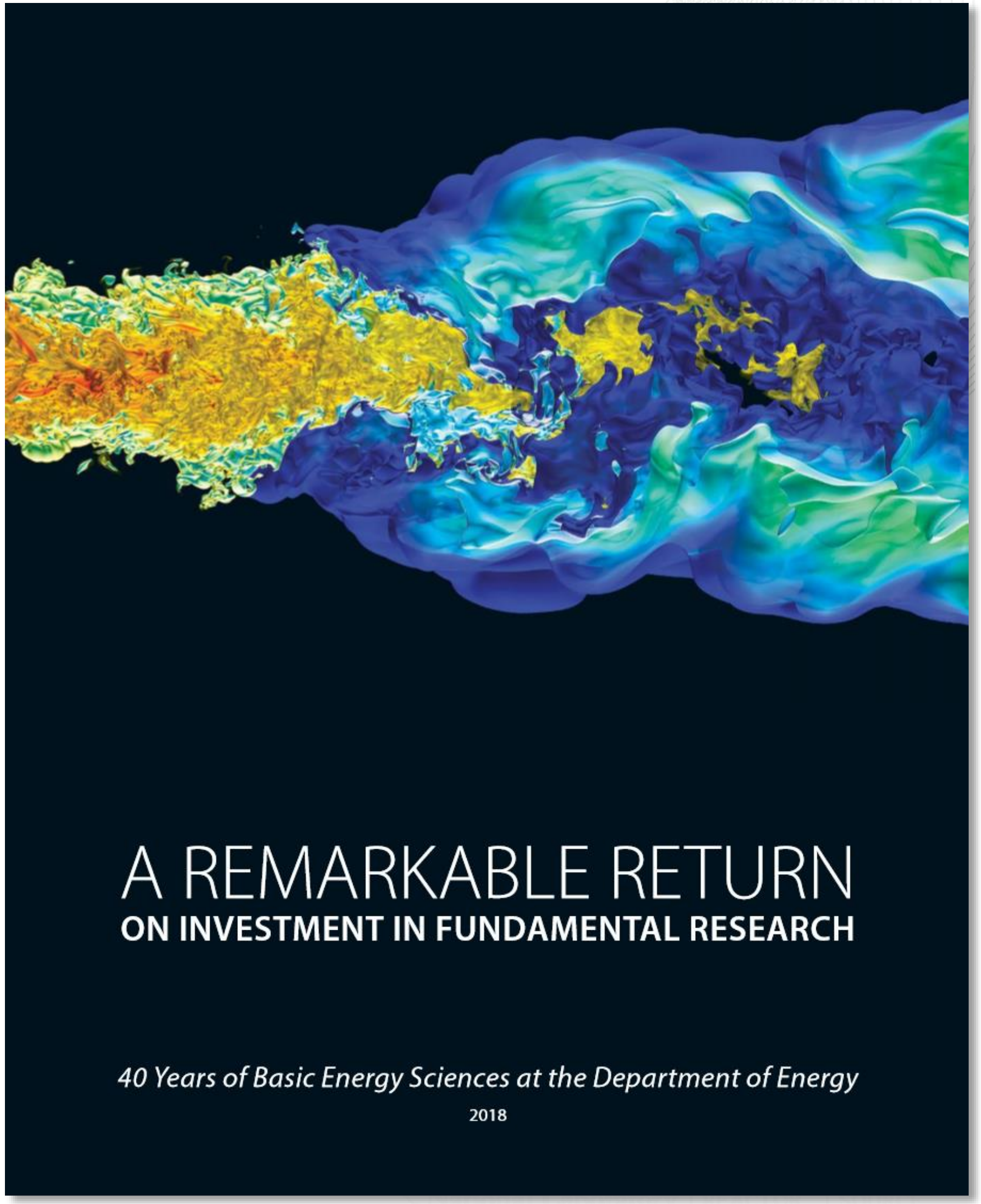
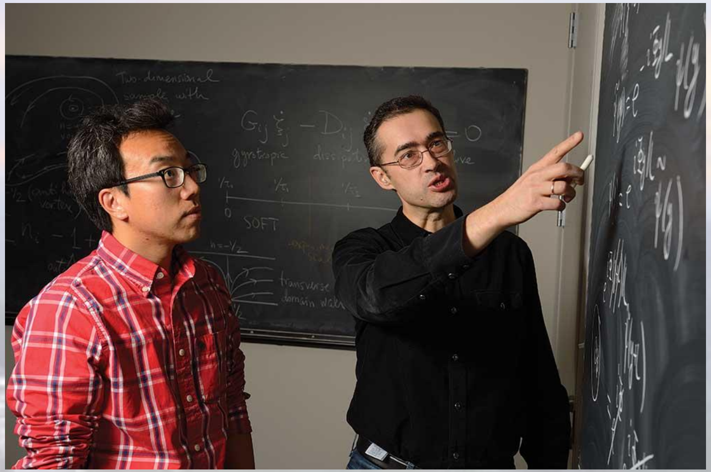


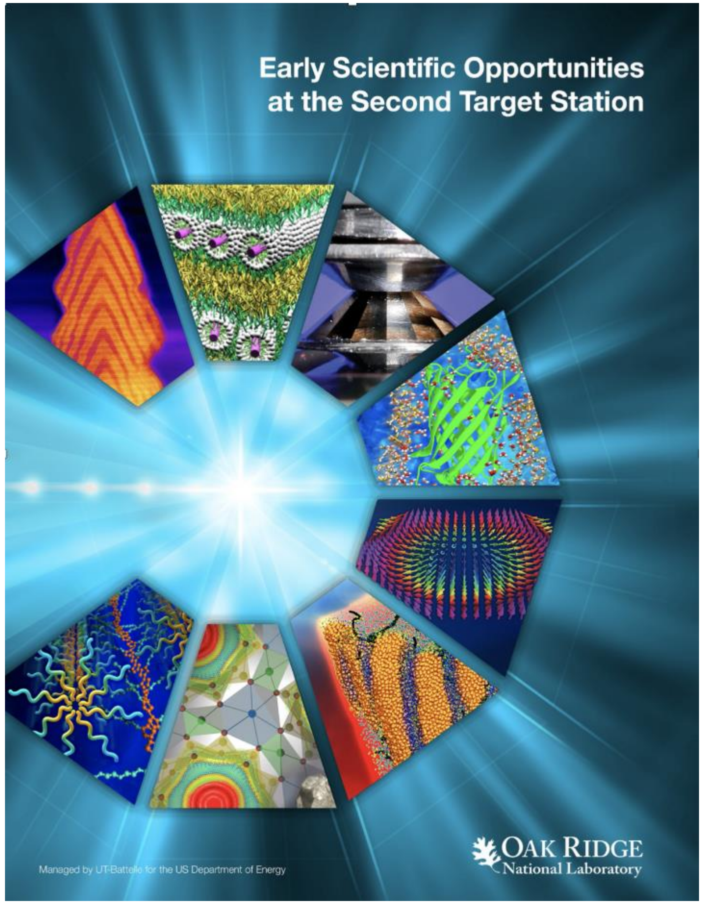
How Neutron Scattering Facilities Work

- Facilities as innovation hubs
  - Science driven by user community
  - Instrumentation advances driven by facilities
  - multi-disciplinary innovative environments
- Output driven by the quality of
  - Materials and ideas from users
  - Neutron Source
  - Neutron instrumentation
  - Sample environment
  - Instrument scientists
  - Primary data analysis
  - Theory and modelling



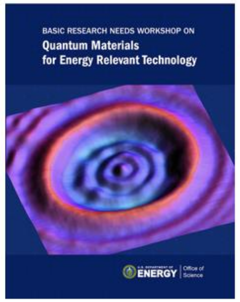
$Pr_2Zr_2O_7$
Koohpayeh

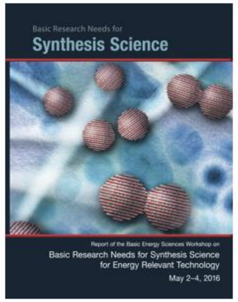
Scientific opportunities at the STS

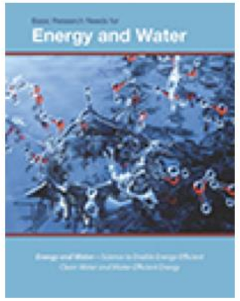


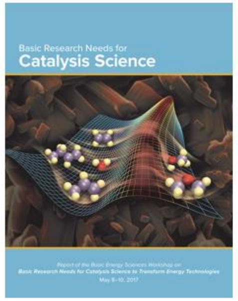
Community workshops 2015-2016

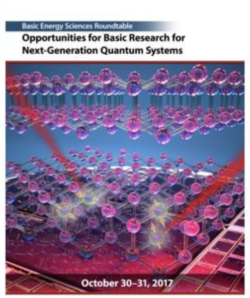
- Emergent Quantum Materials
- Soft Condensed Matter
- Life Sciences
- Materials Discovery, Characterization, and Application
- Neutronic technologies for the STS
- Proposed instrument Concepts

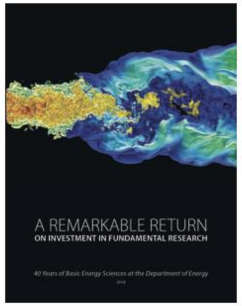






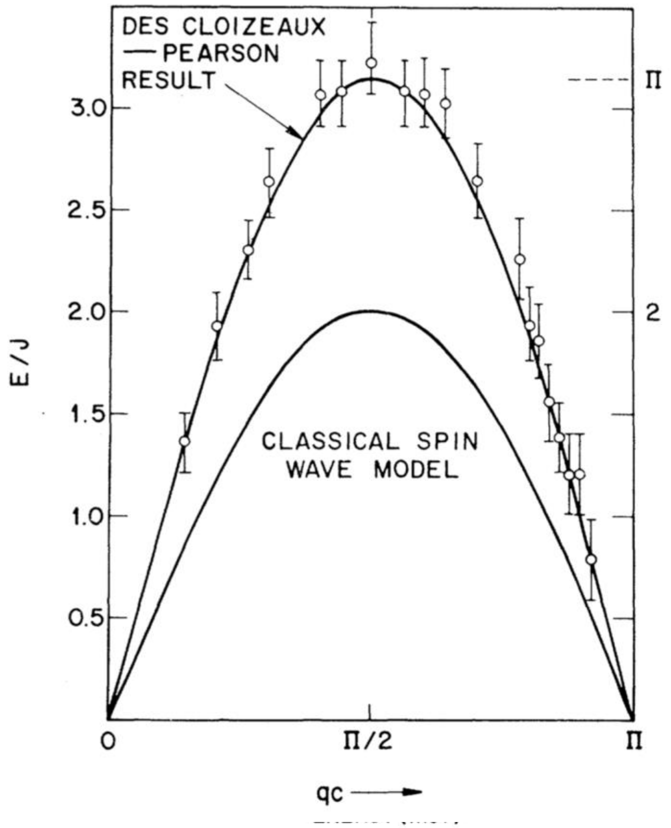




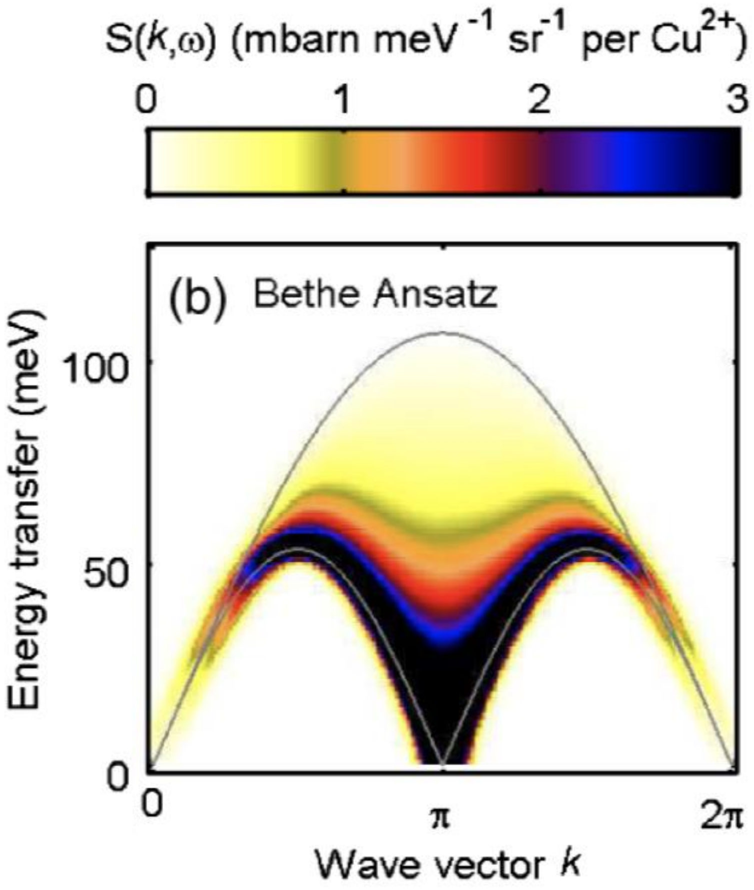


Exotic Quasi-particles in Quantum Magnets

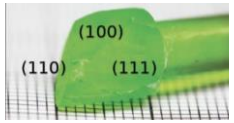
$CuCl_2 \cdot 2N(C_5D_5)$
Endoh, Shirane, Birgeneau et al. (1974)

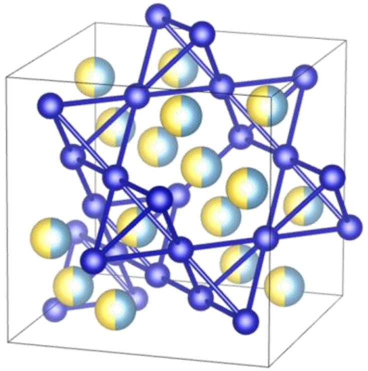


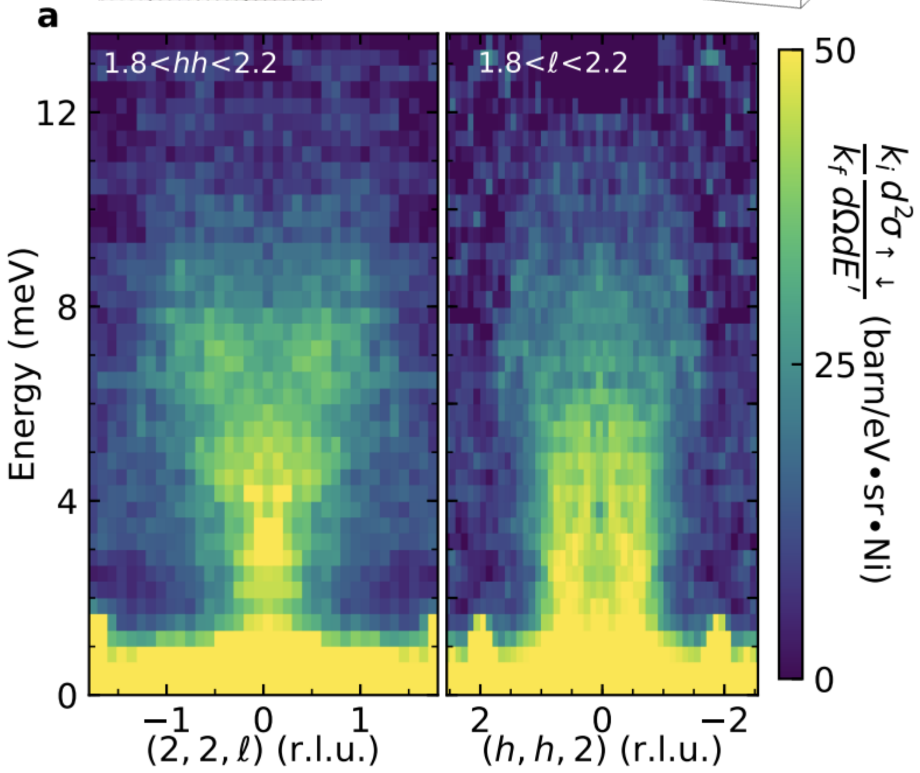
KCuF3
Lake, Tennant, Caux et al. (2013)

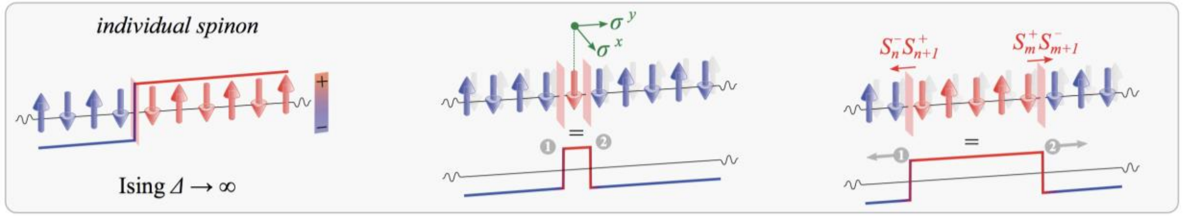


$NaCaNi_2F_7$
Plumb et al. (2018)



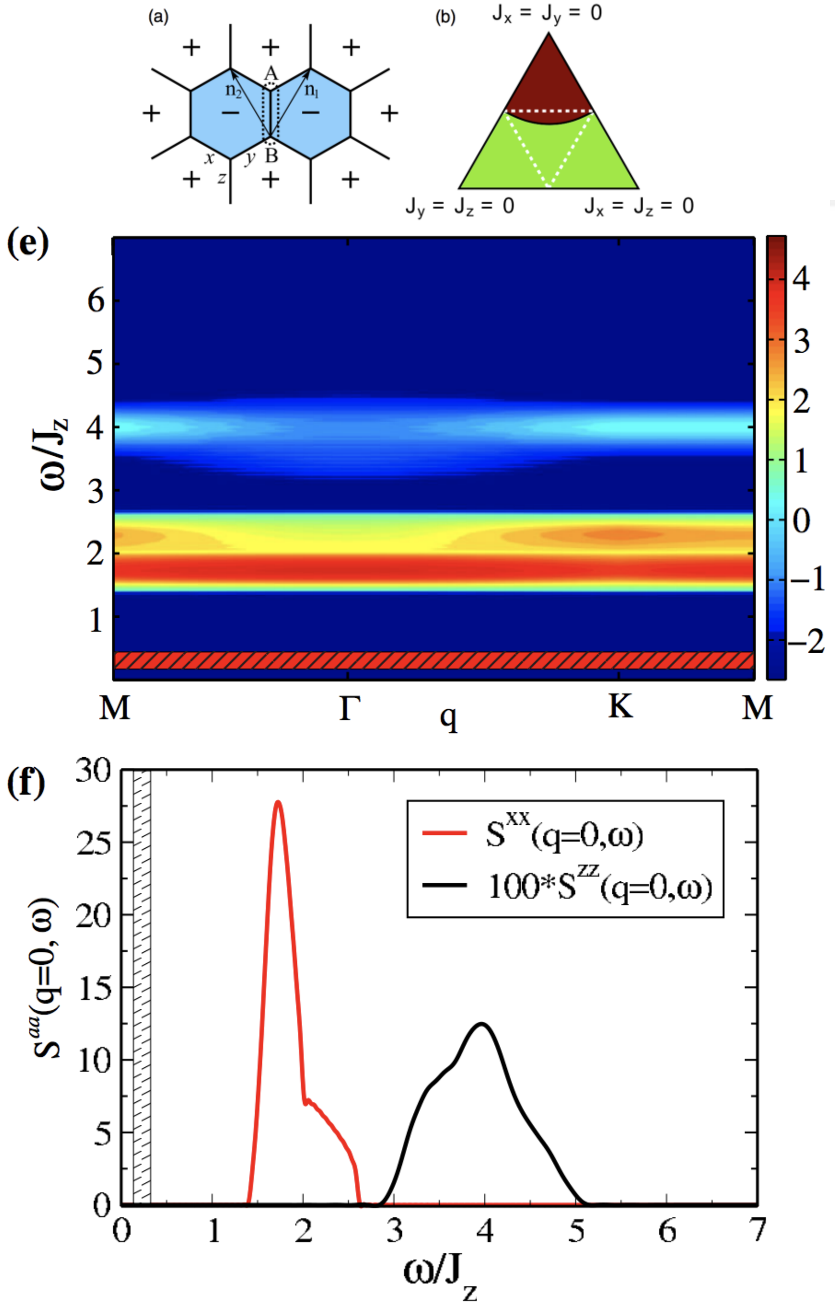




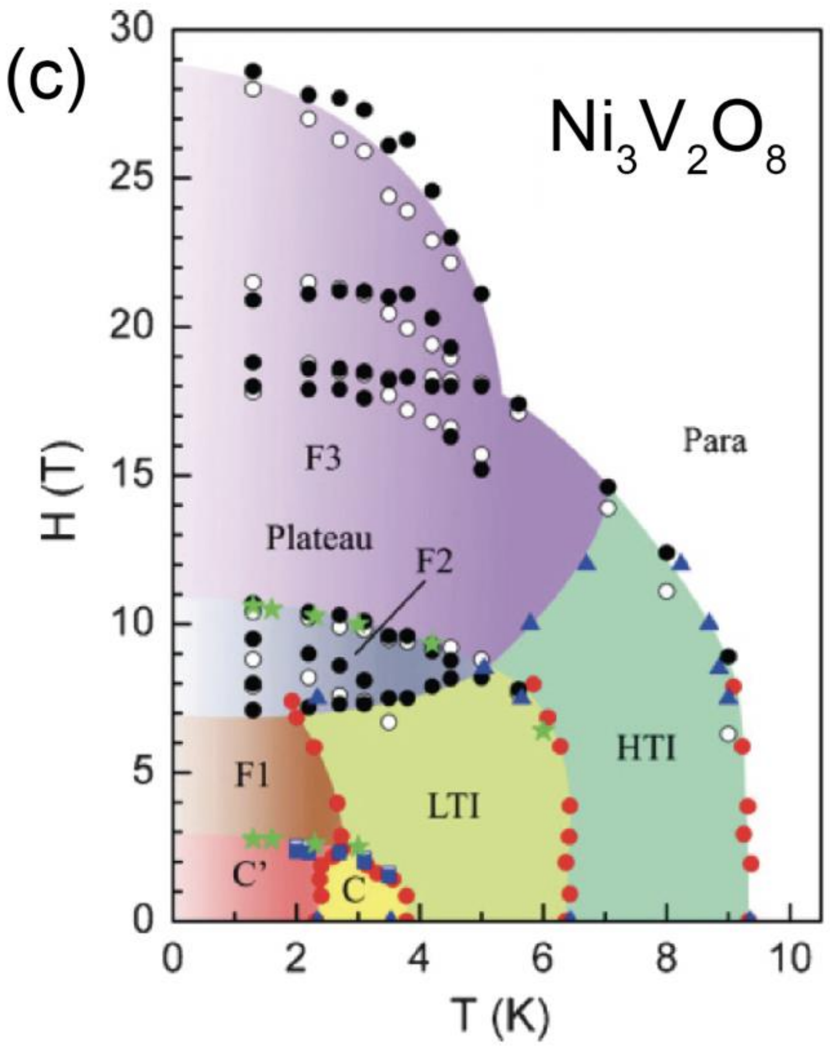


polarized neutrons on HYSPEC-SNS

Spinons, visons, and majoranas in quantum magnets



Probing field driven phases of quantum materials



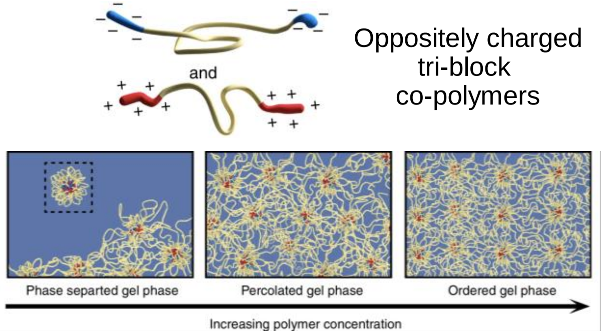
Bright cold neutrons @ STS:

- High efficiency Polarized INS
- Ultra high field scattering
- High pressure INS
- Time evolution beyond equilibrium
- Deep integration with theory and simulation

Soft matter:
Beyond equilibrium and in extreme conditions

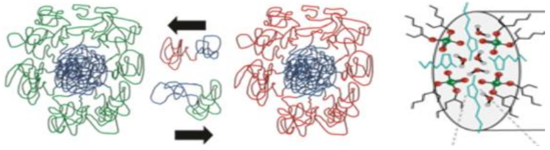
FTS capabilities:
Sensitivity to H/D, non destructive and highly penetrating, dynamic time-scales ~100 ns, time-resolutions ~1 min, limited by weak-signal-to noise

Phase morphologies



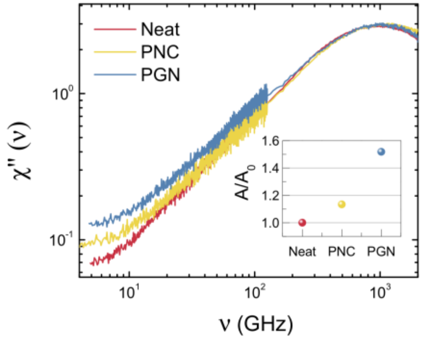
Srivastava et al., *Nature Com.* 2017

Kinetics, functional polymers and micelles



Abney et al., J. *Phys. Chem. Lett.* 2017

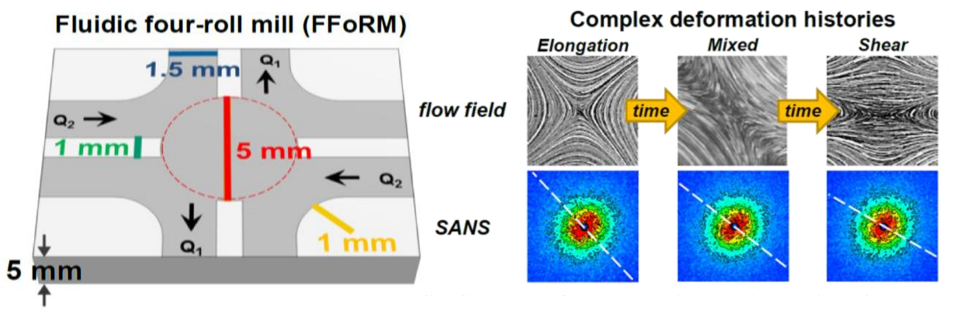
Dynamics & transport

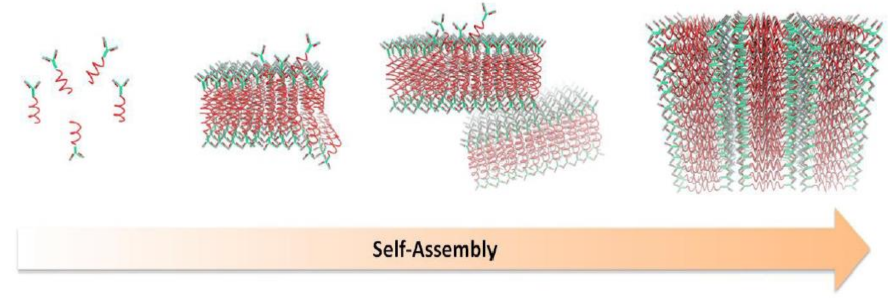


Holt et al., *Phys. Rev. Mat.* 2017

STS capabilities:
dynamic time-scales up to ~1 μs, time-resolutions down to ~10 – 100 ms, single-pulse experiments, simultaneous access to broader length-scales, S/N gains for experiments *in operando* and under extreme conditions

Dynamic assembly and function of hierarchical systems – flow and shear – transport across films and membranes - soft matter under extreme conditions

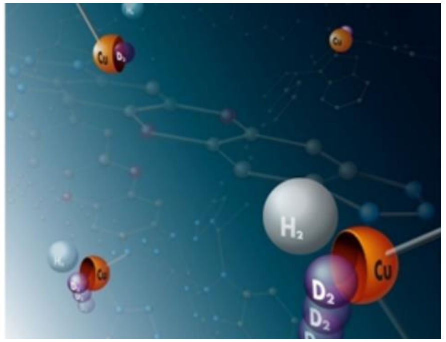




Materials and Chemistry:
In-situ, real-time imaging of synthesis, catalysis, and performance

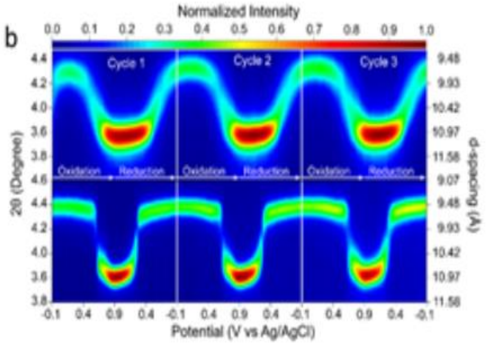
SNS capabilities:
Highly penetrating, sensitivity to light elements, and elements with neighboring Z, vibration spectra from >5 to <400 meV, dynamic time scales ~ ps to ns, diffraction and total scattering, imaging, time-resolutions ~ 1min.

Functional materials



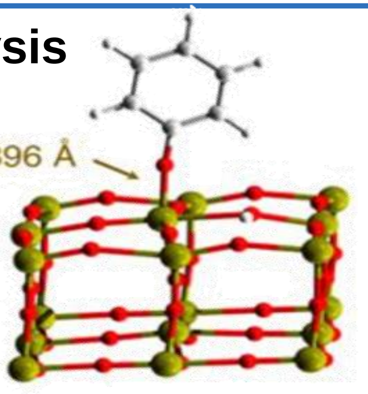
Weinrauch et al. *Nature Com.* 2017

Energy storage



Charles et al. Nature Comm. 2017

Catalysis



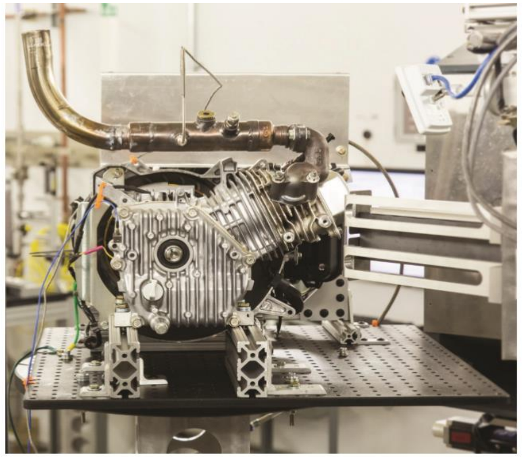
Nb_2O_6

Shao et al., *Nature Com.* 2017

Monitor hierarchical materials across under their extreme operating conditions

STS capabilities:
Large gains in signal-to-noise enable access to extreme environments and time-resolutions ~ 50 ms, simultaneous measurements over broader dynamic range to characterize evolution of structure and chemistry in hierarchical materials

Batteries while discharging



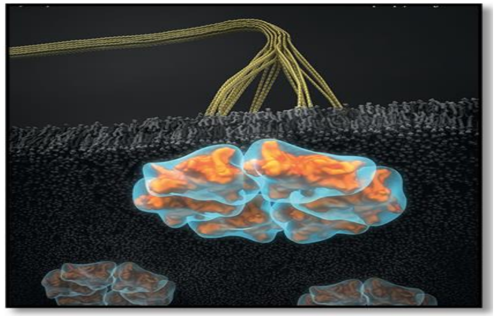
Engines while operating

Hot crystalline turbines

Biological Materials:
Directly following key processes within living systems

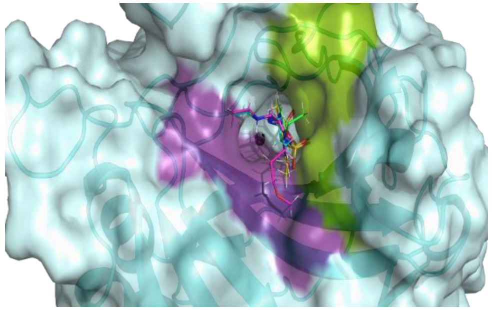
SNS capabilities:
Sensitivity to H/D, non destructive and highly penetrating, dynamic time-scales ~100 ns, time-resolutions ~15 mins, direct visualization of H/D limited by weak-signal-to noise

Complexes and Membranes



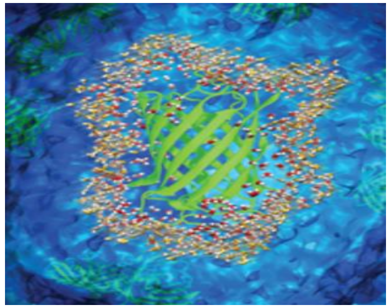
Vandavasi et al., *Plant Phys.* 2016

Enzyme and ligand design



Kovalevsky et al., *Structure* 2018

Dynamics and disorder



Tian et al., *Phys. Rev. Letters* 2018

STS capabilities:
time-scales ~1 μs, time-resolutions 10 – 100 ms, single-pulse experiments, signal-to-noise gains enabling the study of critical process *in vitro* and within living systems, following catalytic reactions

Dynamic assembly and function of complexes – disorder and flexibility – pathogenic misfolding and aggregation

Summary

- BES pioneered fission and spallation neutron technologies
- Operating with high reliability near their design potential, SNS and HFIR form a world-leading facility for neutron scattering studies of materials
- Advanced materials with hierarchical structures and broad band dynamics require more long-wavelength neutrons, higher peak brightness, and broader wavelength ranges
- PPU and STS upgrades will
  - Provide next generation capabilities to accelerate scientific and technological progress
  - Sustain US leadership in an increasingly competitive international landscape of neutron facilities
- World leading STS performance will open new windows on advanced materials:
  - **Quantum Matter:** Broad band dynamics beyond equilibrium and under extreme conditions
  - **Softer Matter:** Image hierarchical structure during self-assembly and flow
  - **Materials Chemistry:** Structure of materials in operating technical systems
  - **Biological Materials:** Imaging the living cell from atoms to membrane proteins

Discussion