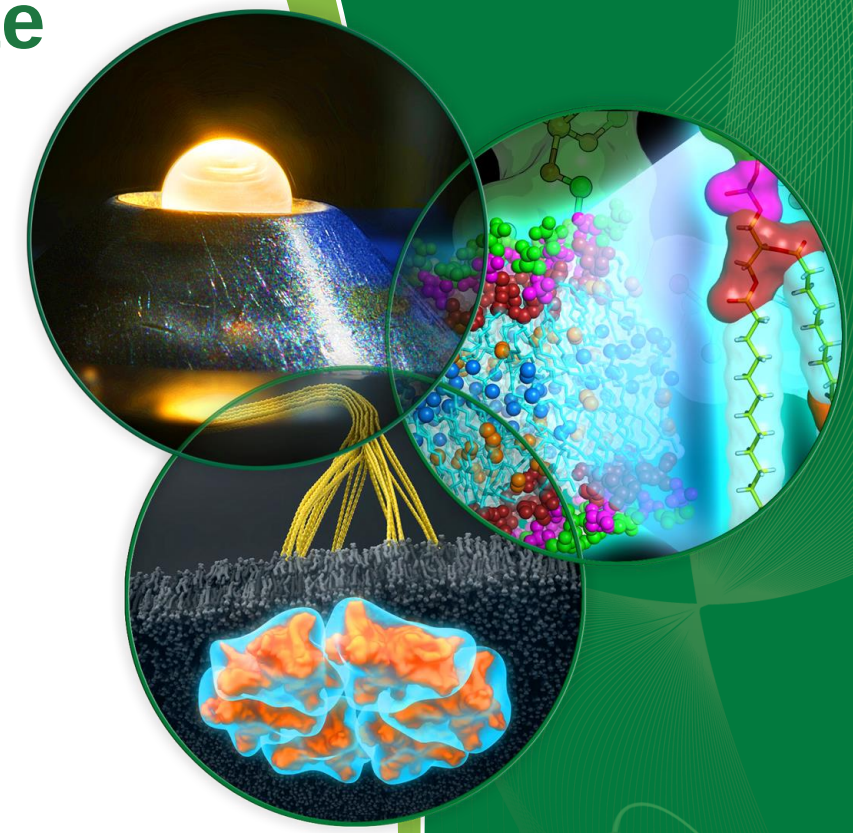
Neutron Sciences
State of the Directorate



Presented to the
Neutron Advisory Board

Paul Langan
Associate Laboratory Director
Neutron Sciences

Clinch River Cabin
Oak Ridge, Tennessee
June 30, 2016

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

We operate two advanced neutron scattering user facilities

High Flux Isotope Reactor (HFIR)
Intense steady-state neutron flux and a high-brightness cold neutron source

Spallation Neutron Source (SNS)
World's most powerful accelerator-based neutron source

U.S. Department of Energy user facilities:
Unique capabilities available through peer review

Headlines since NAB 2015

June 2015

- FY2016 Science Productivity Program steering committee
- Workforce reduction
- DOE triennual review of NScD
- First STS users workshop
- Target 12 sets several new records
- STS project office created
- HFIR celebrates 50th anniversary
- *In situ* plasma processing
- 

- HFIR reaches 1 terawatt-day
- FY2016 budgets announced

February 2016

OAK RIDGE National Laboratory

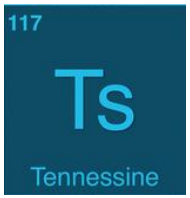
Headlines since NAB 2015

February 2016

Decision to run HFIR for 7 cycles

Software scientists embedded on beamlines and data plan developed

UT gives JINS a new name: Shull Wollan Center



Annual user publications for 2015 pass 400

SNS celebrates 10th anniversary

FY2017 Science Productivity Program steering committee

Rebalancing HFIR and SNS staff

BESAC facilities prioritization report

Today

2008– 2016
10,000+ proposals submitted to General User Program

OAK RIDGE National Laboratory

Our neutron sources are operating well

SNS: Operating at 1 MW since 30 March 2016; 1 spare target on hand

- Target installed in late March
  - Excellent data from 2nd generation target instrumentation
  - Record speed for target change: 8 days
- Controlled experiments on current and next target at fixed beam power (1/1.2 MW) to quantify cavitation damage erosion rates

HFIR: Operating well after very successful long outage

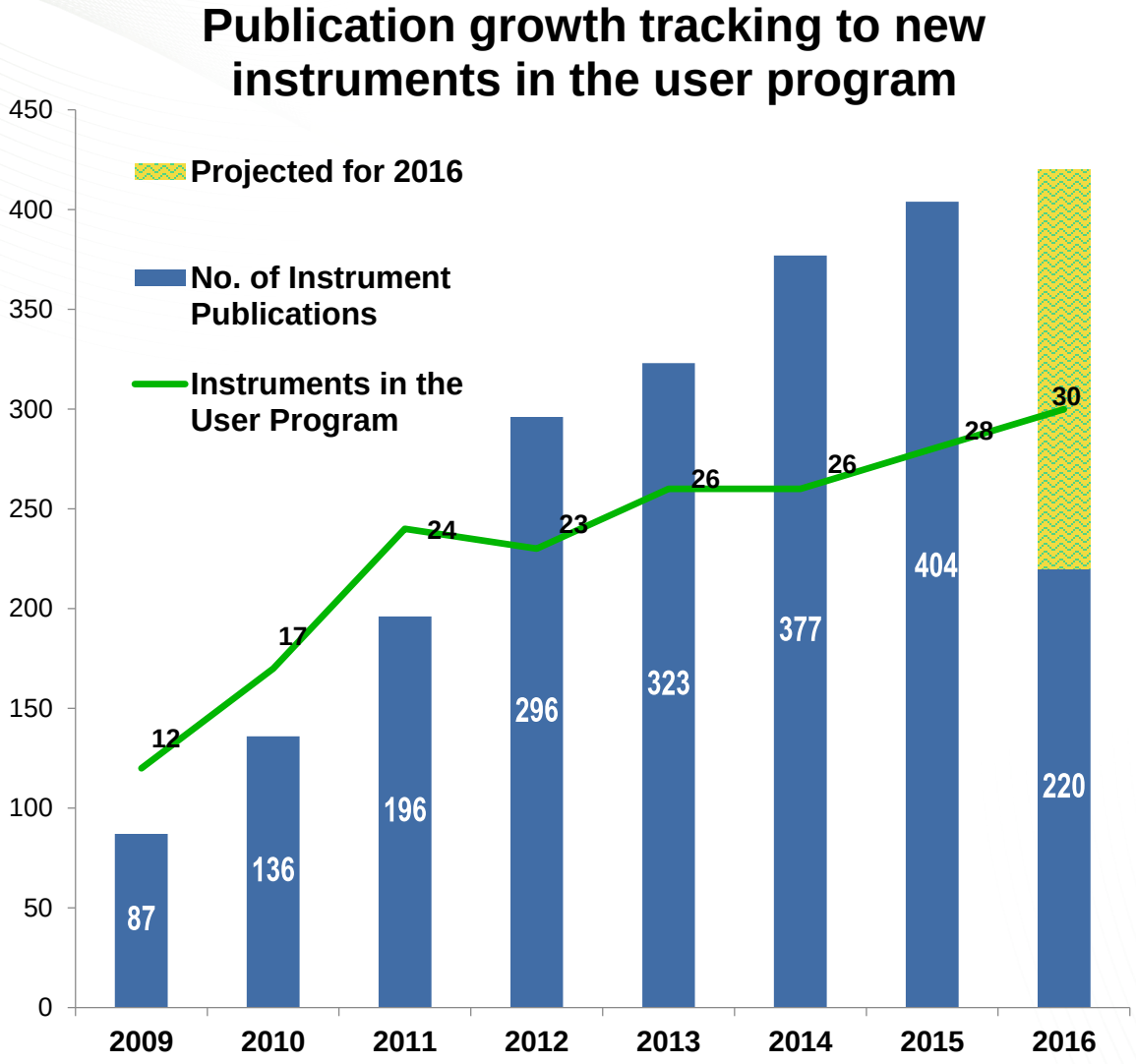
- Cooling towers rebuilt, control rod drives rebuilt, new safety plates
- 1 million MW days of operation achieved
  - Equivalent to running every day at 85 MW for >30 years
- Availability goal increased to 7 cycles

SNS	Goal	As of 5/31/15
Unique users	780	696
Predictability	90%	91.7%
Availability	90%	84.3%
Operating hours	5,000	3986.2

HFIR	Goal	As of 5/31/15
Unique users	340	281
Predictability	90%	100%
Availability	7 cycles	4 cycles
Operating hours	3,700	2,376.8

All other systems operating well; FY16 availability excluding target failures is ~92%

Neutron scattering upgrades will drive continued growth in productivity



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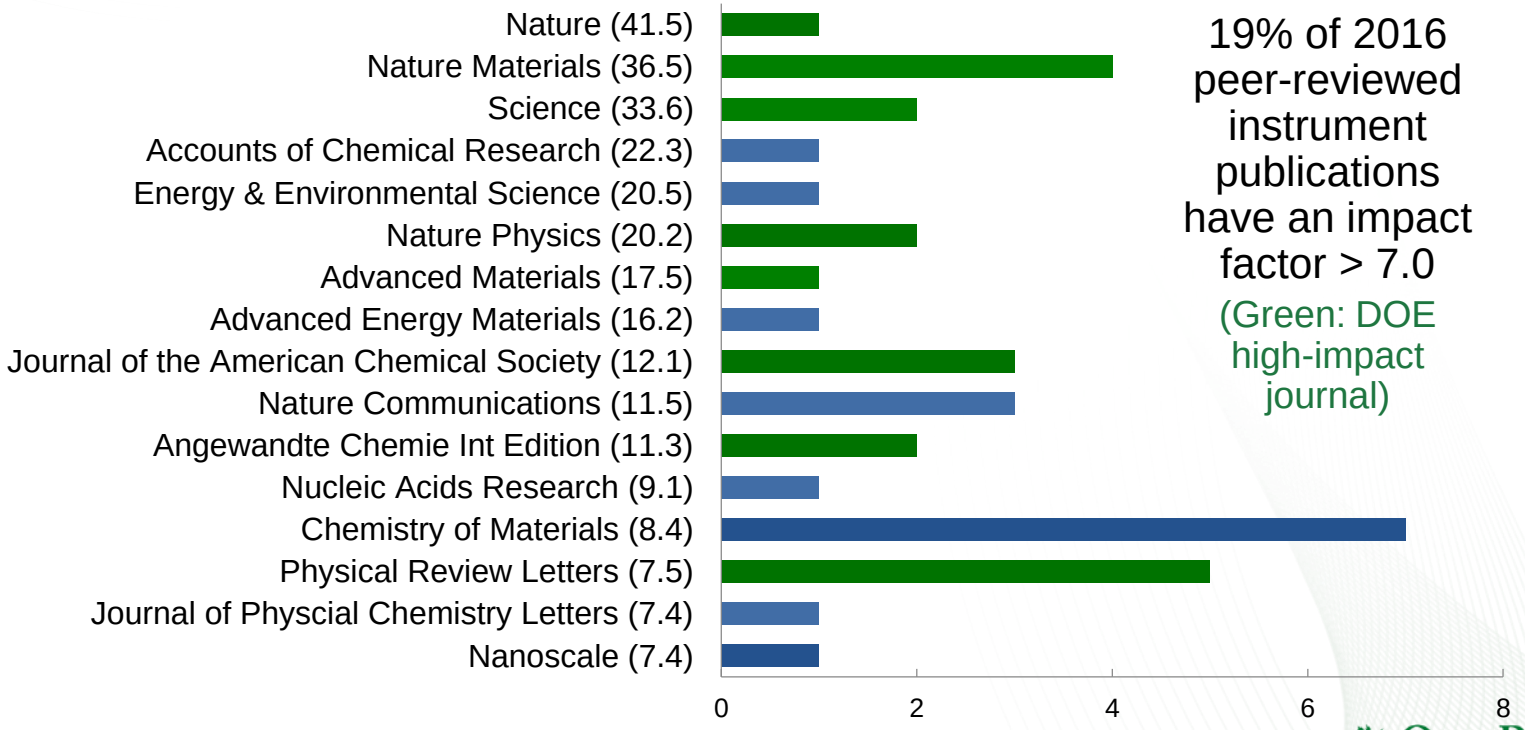
The proportion of high-impact publications is growing

Publications by Facility	CY2016 to date	Total CY 2015	Total CY 2014
HFIR Instruments only	5	9	6
SNS Instruments only	13	19	20
Both HFIR and SNS instruments	3	2	3
NScD non-instrument	7	11	12
Total	**26**	**41**	**41**



19% of 2016 peer-reviewed instrument publications have an impact factor > 7.0

(Green: DOE high-impact journal)

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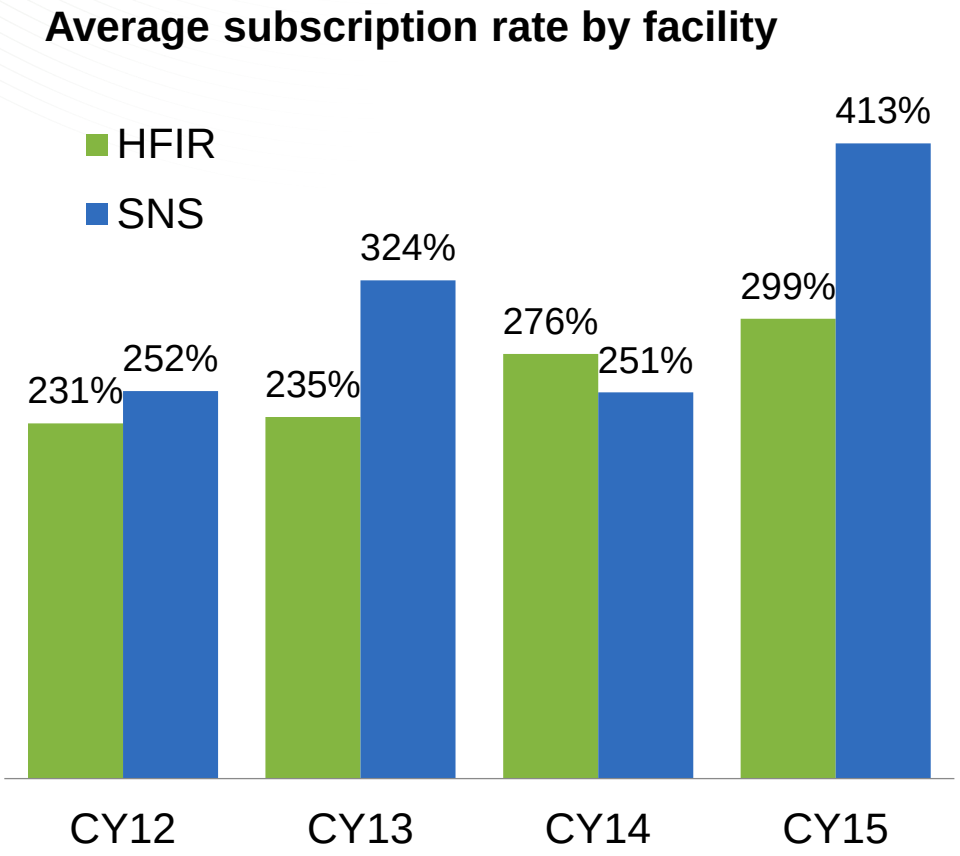
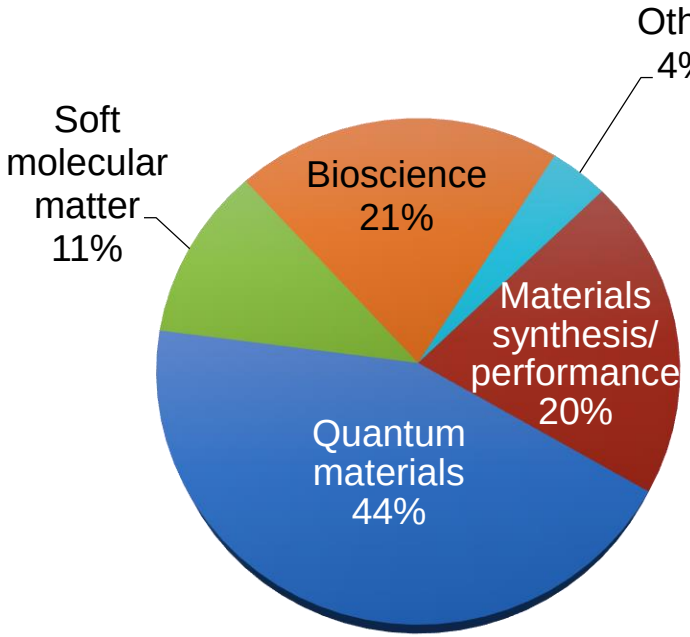
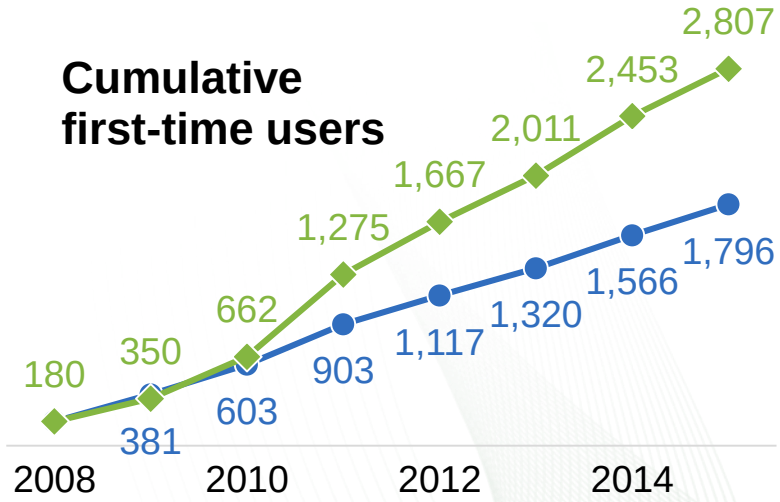
Our community is growing and instruments continue to be oversubscribed







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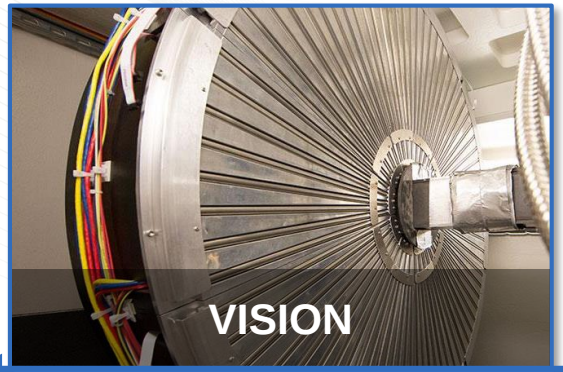
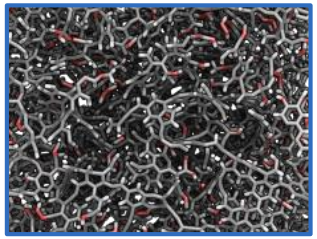
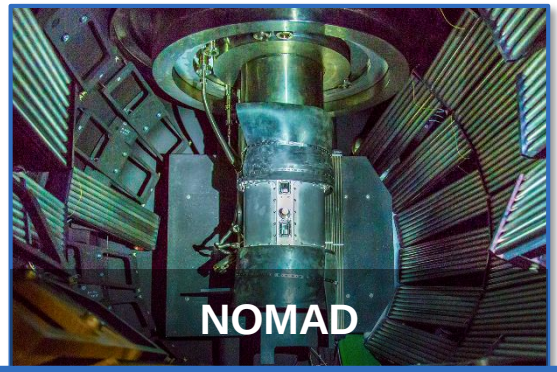
We are delivering world-leading neutron scattering instruments



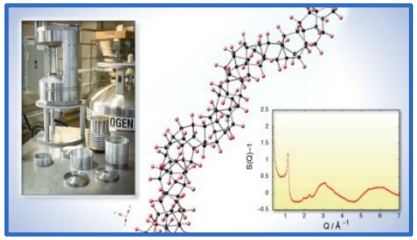
Neutron-derived vibrational densities of states and pore size distributions reveal organic matrix in gas shale critical to gas production potential



Bousige et al. *Nature Materials* (2016)

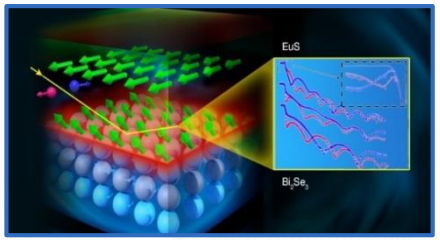


Neutrons reveal new class of material: Diamond nanothreads synthesized from benzene at 20 GPa



Fitzgibbons et al., *Nature Materials* (2015)

Neutrons key in discovering high-temperature topological insulator by proximity coupling



Katmis et al., *Nature* (2016) in press

OAK RIDGE National Laboratory

We engaged the research community to develop a strategic science plan

Near- and long-term goals will help us realize our vision

Science priorities

Defined through broad community engagement

- Soft molecular matter
- Quantum materials
- Materials synthesis and performance
- Biosciences

Near-term focus

Maximize scientific impact at SNS and HFIR

- Sustain and improve neutron production at SNS and HFIR
- Complete and optimize neutron scattering instruments and develop related innovative capabilities and technologies
- Build out open beam lines on first target station (FTS)

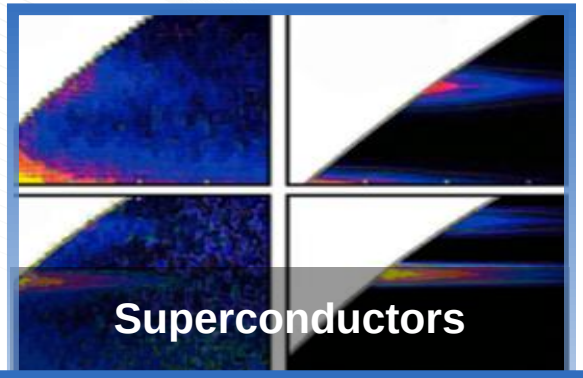
Long-term focus

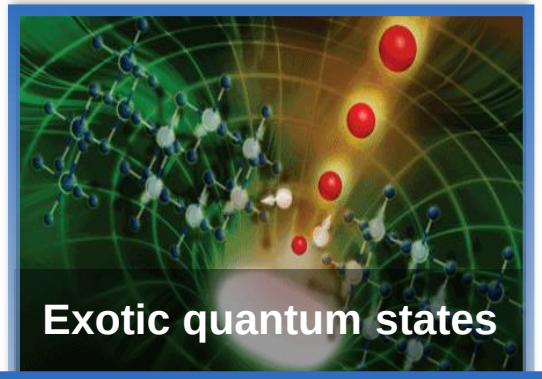
Addressing emerging grand challenges that will dominate next two decades

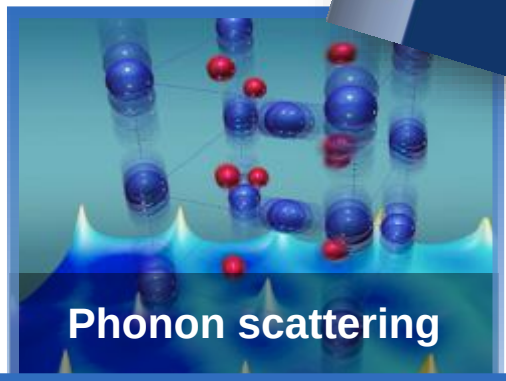
- Design, build, and commission a second target station (STS) for SNS, supported by a proton power upgrade (PPU)
- Optimize science across three complementary sources, providing unrivalled capabilities

OAK RIDGE National Laboratory

Science priorities drive investments for quantum materials



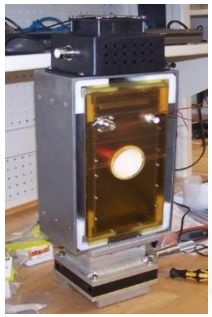




High magnetic fields, low temperatures, high pressure, spin manipulation

Integration with theory and modelling, focusing optics

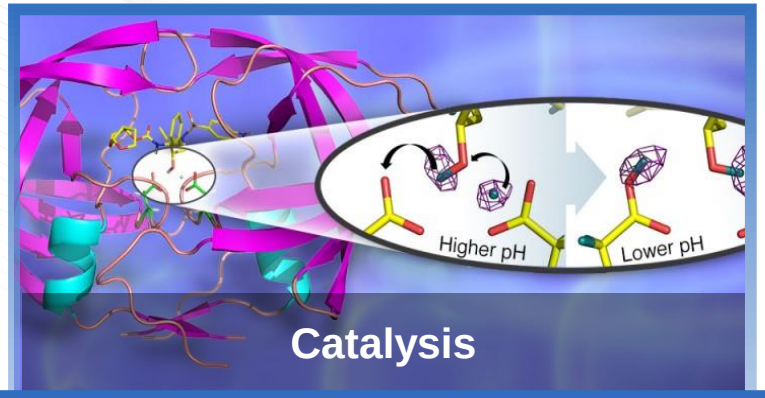
Larger detector coverage, sample changers

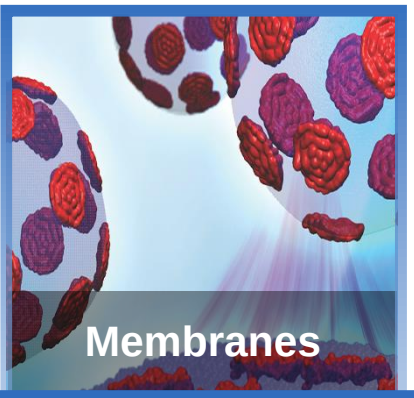


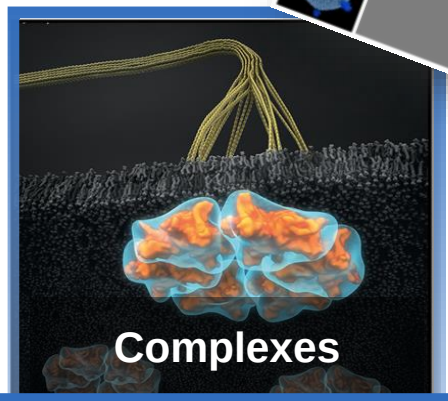
Neutrons are a vital tool for materials research that provide information that cannot be obtained by other techniques

OAK RIDGE National Laboratory

Science priorities drive investments for biosciences







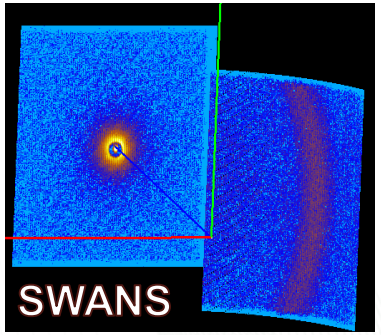
Dynamic nuclear polarization

Deuteration and molecular biology

Integration with theory and modelling

Informed by data from multiple techniques

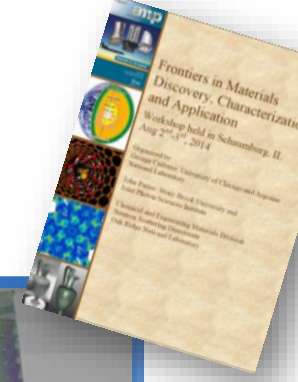
Multiscale measurements

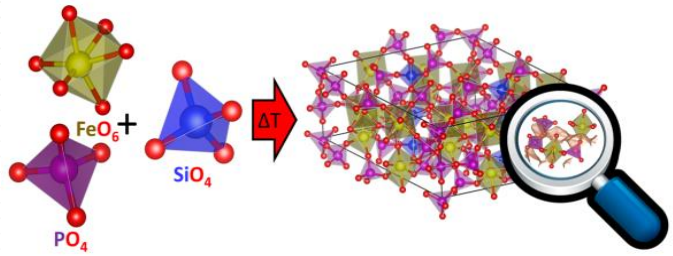


Neutrons are a vital tool for materials research, providing information that cannot be obtained by other techniques

OAK RIDGE National Laboratory

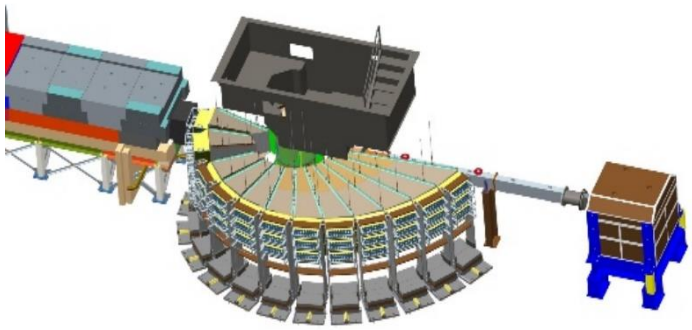
Science priorities drive investments in materials and chemistry

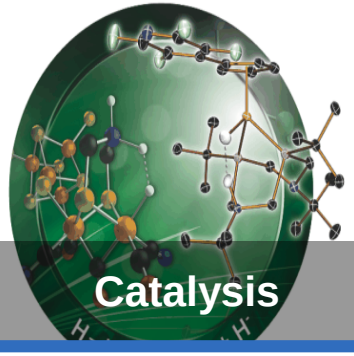




Energy storage

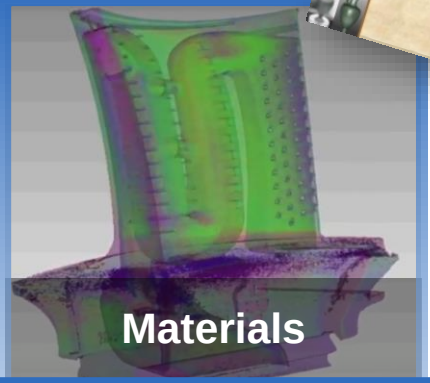
Fast in situ experiments





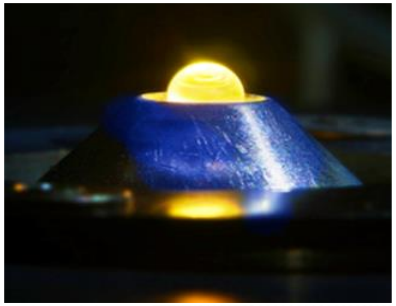
Catalysis

Real-time calculations



Materials

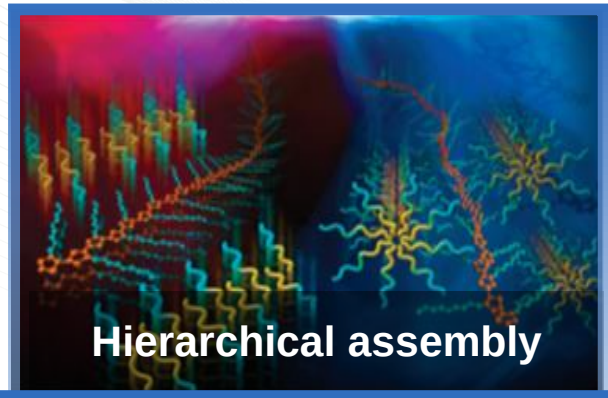
High temperature, pressure and load

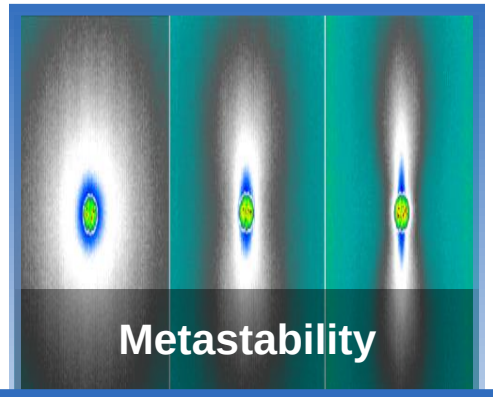


Neutrons are a vital tool for materials research, providing information that cannot be obtained by other techniques

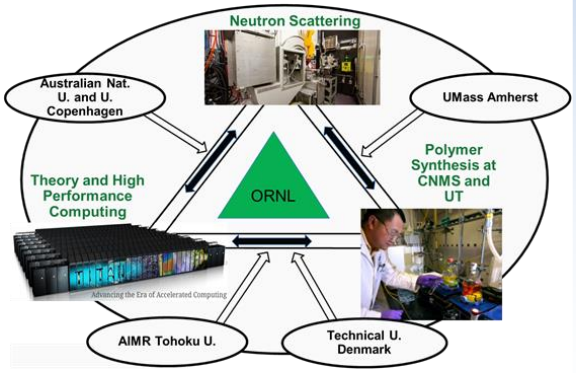
OAK RIDGE National Laboratory

Science priorities drive investments in soft matter

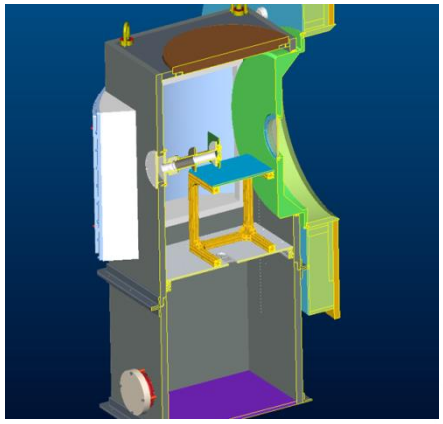




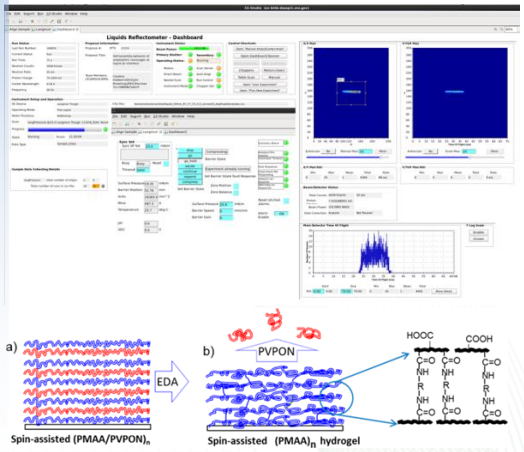
Combining synthesis, modeling, and experiment



Advanced sample environments



Science driven interfaces



Neutrons are a vital tool for materials research that provide information that cannot be obtained by other techniques

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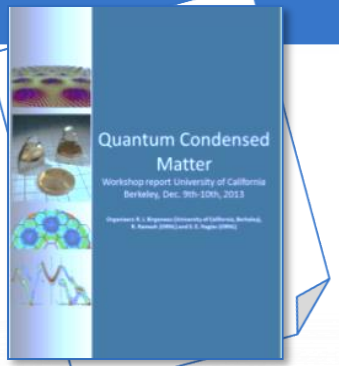
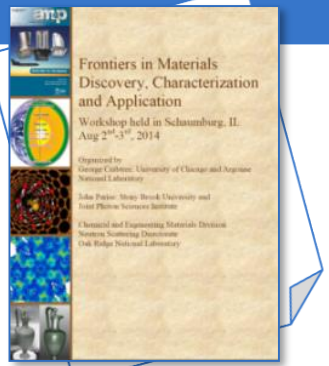
New areas of scientific growth

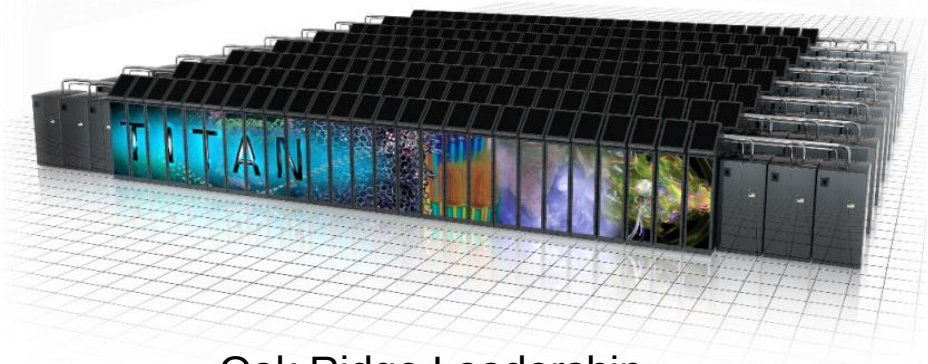
Industry, engineering, and additive manufacturing

Nano-structured and disordered materials

Soft matter







Oak Ridge Leadership Computing Facility

Center for Nanophase Materials Sciences

DOE conducted a triannual review of neutron sciences in August 2015

Informal feedback from DOE sponsors and reviewers

There was a dramatic contrast to previous reviews with a strong shift in focus to scientific productivity

The SNS and HFIR are transforming into a first class facility

It is clear that there is strong support from the Lab and that ORNL is really behind Neutron Sciences

Triennial Review recommendations

- Continue to develop Science Productivity Plan, define actions, and integrate into operating plans
  - A. Bring number of staff supporting SNS beamlines down to international norms
  - B. Rebalance resources between SNS and HFIR to ensure continued HFIR scientific productivity
- Fix problems with SNS work planning tools
  - A. Make data analysis and reduction a high priority
  - B. Embed software staff in instrument research groups
  - C. Provide DOE with periodic reports
- Instruments
  - A. Fix the problem with the productivity of powder diffraction instruments
  - B. Increase fraction of high-impact publications from all SNS and HFIR instruments
- Targets
  - A. Place maximum priority on target performance
  - B. Replace targets early to maximize operating hours
- Run HFIR for 7 cycles
- Rebalance resources for operations and new developments to address high-priority (1) instrument upgrades and (2) vital upgrades of accelerator components and reactor complexes
- Develop a plan to take full advantage of co-location of CNMS and HFIR/SNS

Responses to your 2015 recommendations

Recommendation/comment	Response
Expand science productivity pilot program	Expanded across all instruments; $10M focused on improvements; initiating external reviews; updated strategic science plan and vision
Don't attempt regular 1.4 MW before commissioning new RFQ	Developed plan for systematic ramp-up to 1.4 MW over next 2 years
Increase broader user community in planning and strategic development for STS and existing sources	Initiated SHUG on site meeting; expanded user group meeting and STS workshop, town hall meetings at conferences, national science tour
Increase science productivity and impact and set publication goals	Number of publications and their impact have increased; strategic science plan includes identification of improvements to realize maximum publications rates on instruments
Give utmost priority to computing strategy and focus on immediate needs	Plan being executed to address day-to-day need of users for data collection, reduction and analysis; software developers embedded on instruments
Develop a comprehensive strategy for 3 source complex and a clear science vision	Laboratory communications team engaged to develop 3 source communication strategy; science vision continues to be developed

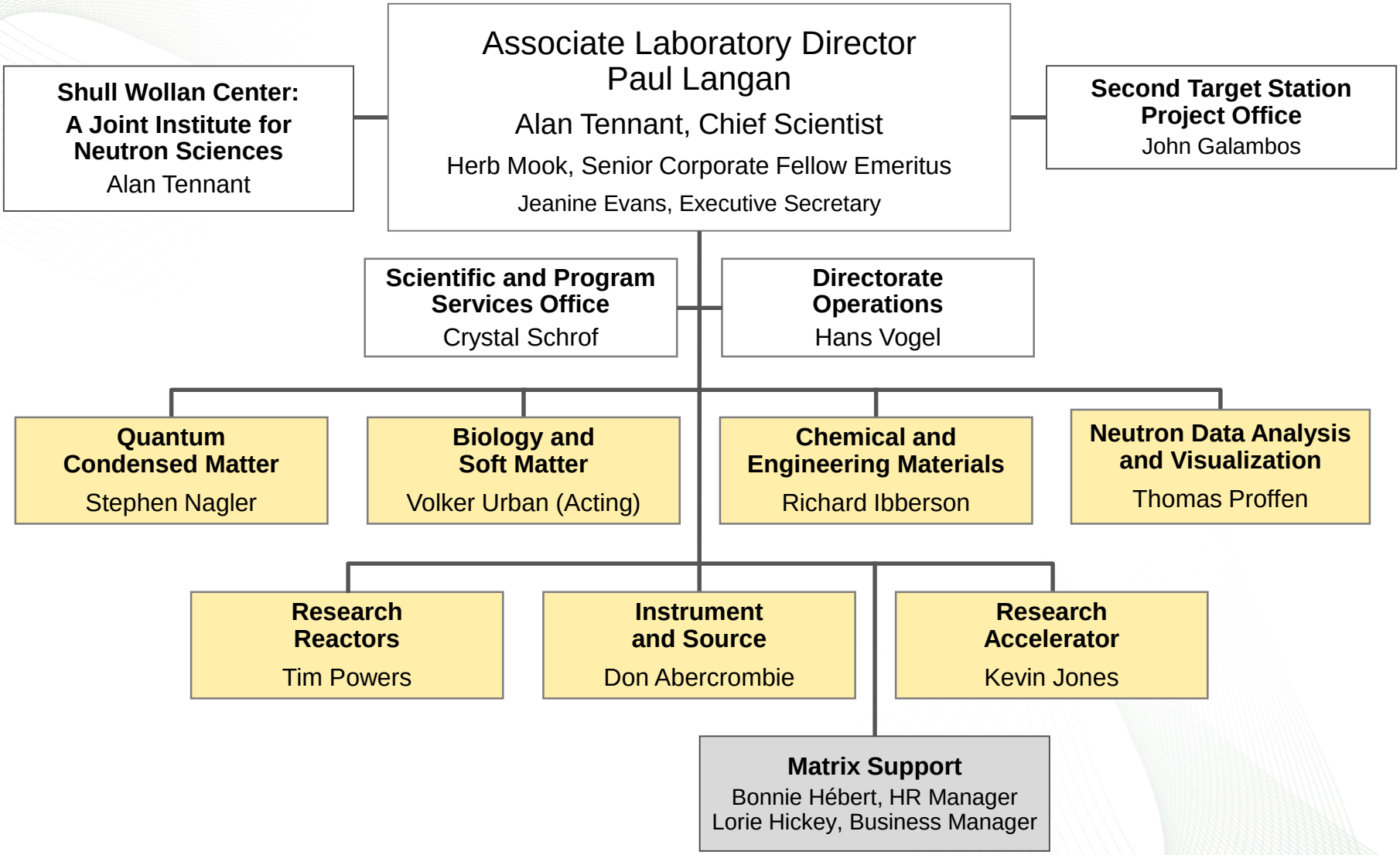
Our budget has been increased and includes initial funding for STS

FWP	FY 2015 ($M)	FY 2016 ($M)
High Flux Isotope Reactor	$61.6*	$63.4
SNS Research Accelerator	$90.3**	$91.0
Accelerator Improvement Projects	$1.5	$2.0
Instrument and Source	$28.5	$28.2
Neutron Scattering Sciences	$62.4	$67.0
Second Target Station (STS)	–	$10.0
Total	**$244.3**	**$261.6**

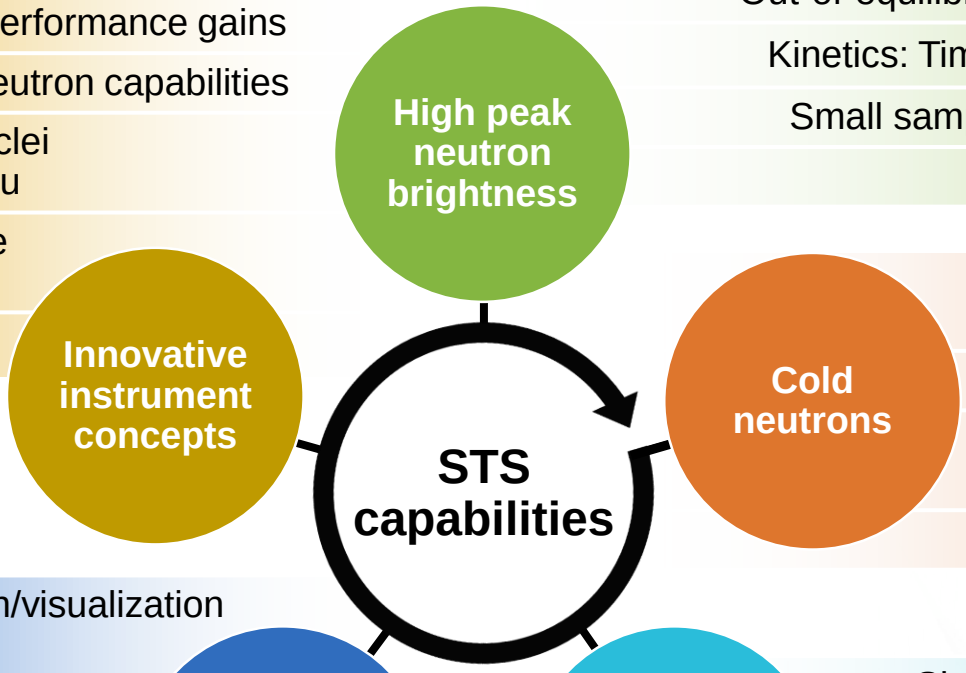
*Includes $3M reallocation from SRS fuel assemblies and $0.6M of reserves for fuel

**Includes $1.3M reallocation of SING II for heavy water

We established an STS office in the Neutron Sciences Directorate



Innovative STS design enables new science to meet BES needs



- 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

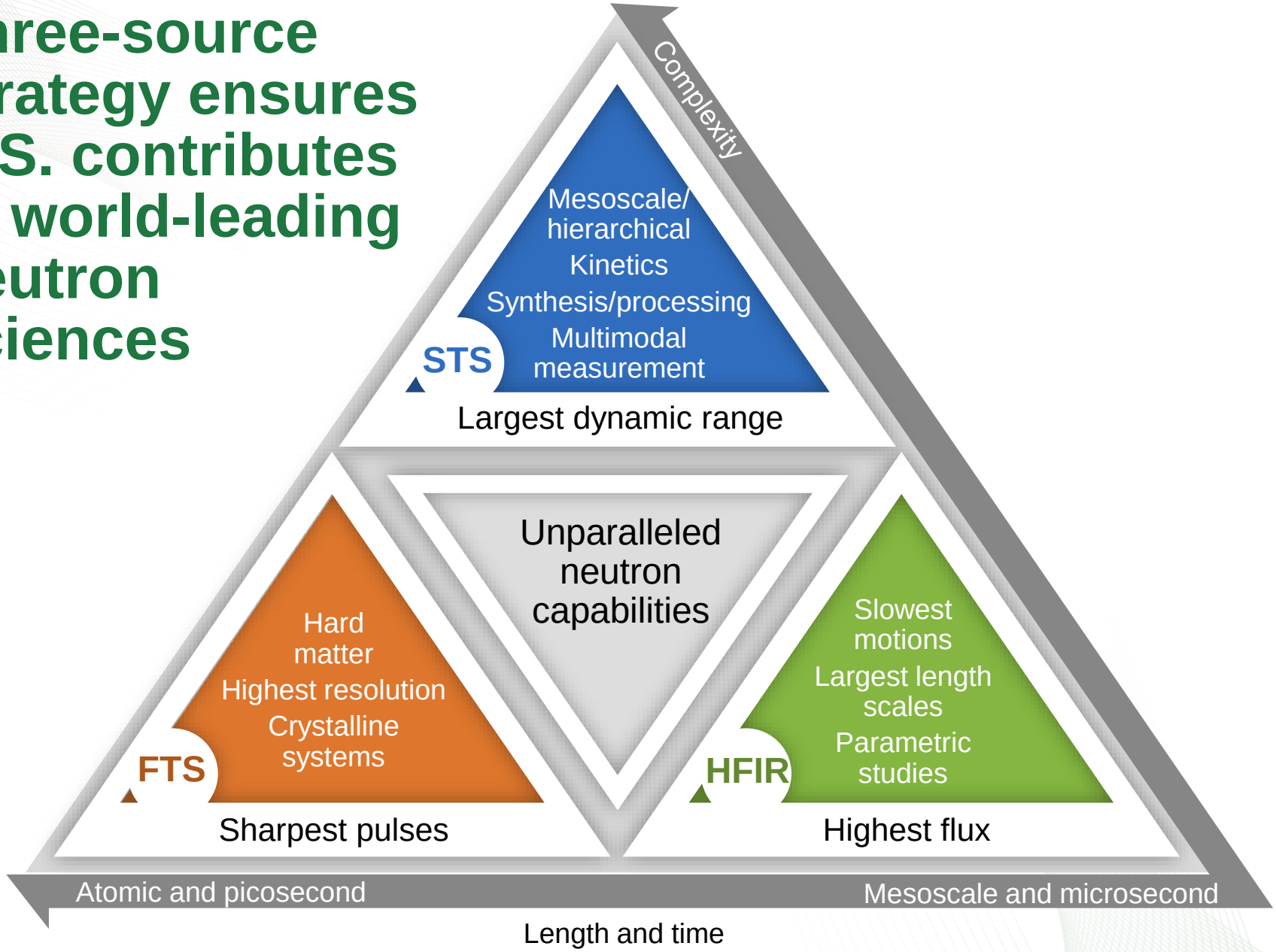
- High-throughput – in situ sample synthesis
- Out-of-equilibrium behavior phenomena
- Kinetics: Time-dependent phenomena
- Small samples – microspot scanning
- Parametric studies

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

- 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

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

Three-source strategy ensures U.S. contributes to world-leading neutron sciences



OAK RIDGE National Laboratory

Main findings of BESAC review

The SNS in combination with HFIR makes Oak Ridge National Laboratory one of the world leading experimental facilities for neutron experiments. However, the European Spallation Source, now under construction in Sweden, will soon eclipse the SNS first target station. The Proton Power Upgrade (PPU) and Second Target Station (STS) at the SNS has the potential to provide a pulsed neutron facility that remains world leading. As such the

PPU and STS are considered to be "absolutely central to contribute to world leading science".

Questions exist as to the detailed design and implementation of the STS and how the proton pulses from the PPU are distributed between the first and second target stations …

Establish a review panel to make a detailed evaluation and recommendations on the proposed designs

… charged with detailed analysis of the technical issues such as those related to the STS repetition rate and pulse length.

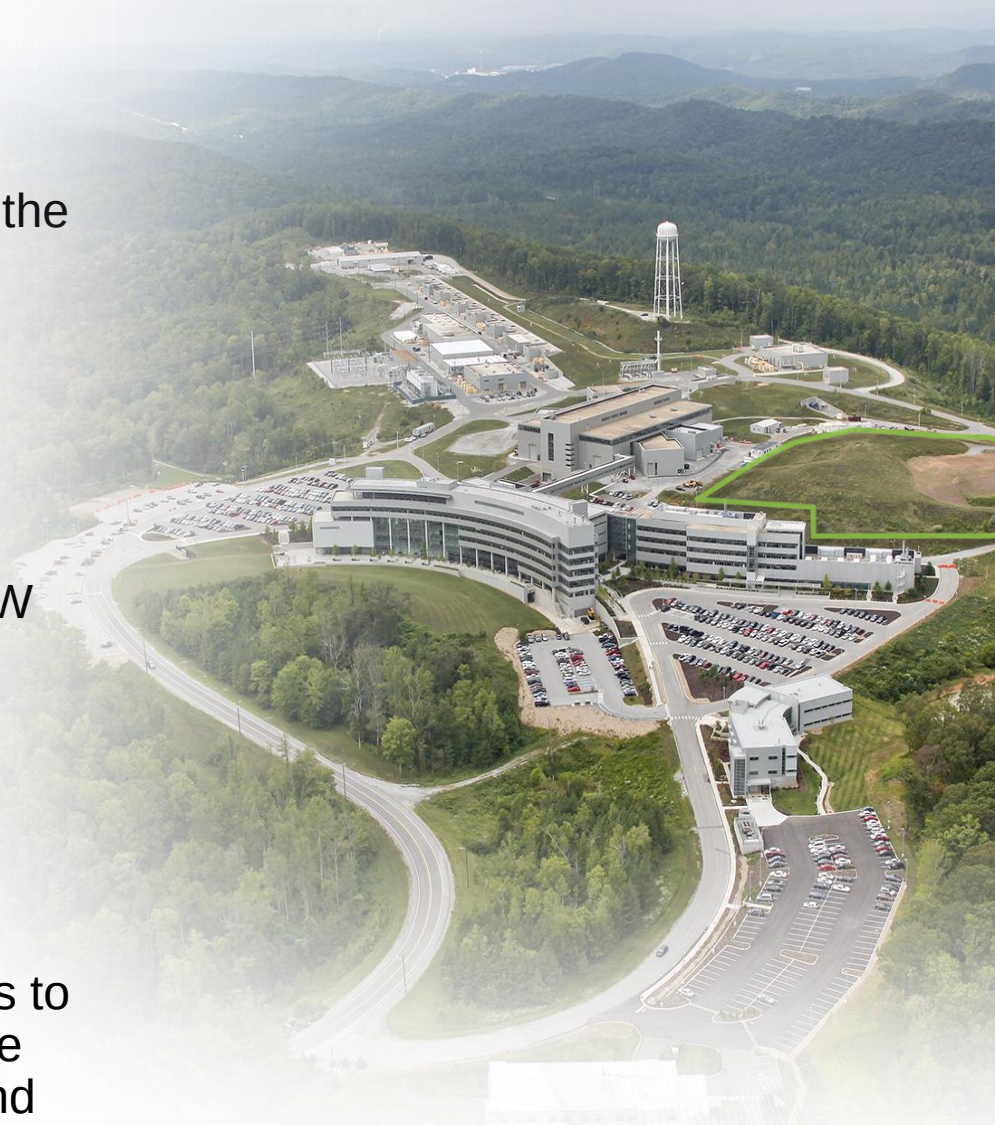
Main recommendations

- Establish a review panel to make a detailed evaluation and recommendations on the proposed designs - detailed analysis of the technical issues such as those related to the STS repetition rate and pulse length.
- Work closely with the neutron science user community to develop the most exciting and robust set of “first experiments”
- Develop more robust targets for the first target station that can fully utilize the proposed SNS-PPU.
- Build-out the experimental stations for the first target station a priority.

Charge to NAB 2016

We seek your feedback and guidance in the following two areas:

- **First Target Station:**
  - Our path to improved scientific productivity
  - Our plans to achieve and sustain reliable operation of SNS at 1.4 MW beam power, improve target predictability and reliability
  - Our plans for improved and new experimental stations.
- **Second Target Station:**
  - Our approach to defining a process to conduct a detailed evaluation of the proposed designs for SNS-PPU and SNS-STS.



Questions