Update on Neutron Sciences at ORNL

Presented to

Basic Energy Sciences Advisory Committee (BESAC)

Presented by

Paul Langan
Associate Laboratory Director
Neutron Sciences

February 27, 2015
North Bethesda, Maryland

OAK RIDGE National Laboratory

BES investment has created 2 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

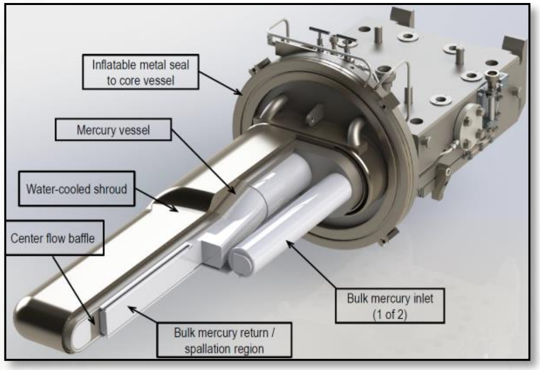
SNS and HFIR met all goals in Fiscal Year 2014

HFIR

- Delivered 3682 production hrs for users over 6 cycles
- 100% predictability
- Operated at 85 MW
- Completed 50 cycles with cold source

SNS

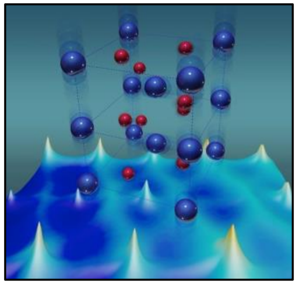
- Delivered 4424 production hrs for users at 94.1% availability against planned hrs
- Operated at ~1.0 MW and 60 Hz
- World record 1.4 MW for pulsed linac
- Developed plan to extend target life-time



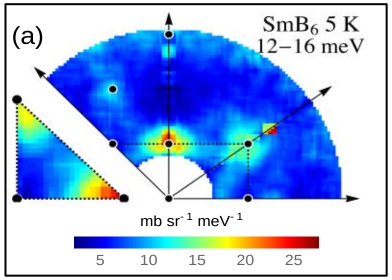
Science program

- Supported 893 unique users at SNS and 453 unique users at HFIR
- Over 900 proposals received during last proposal call setting a new facility record
- HFIR is also an exceptional resource for materials irradiation and neutron activation analysis and continuing mission in isotope production

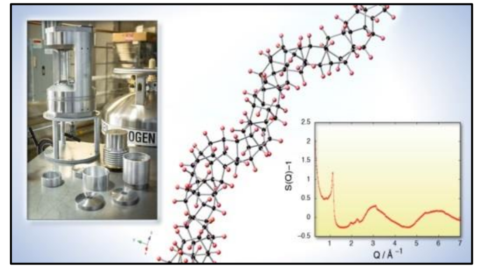
The HFIR and SNS user program is delivering high impact science



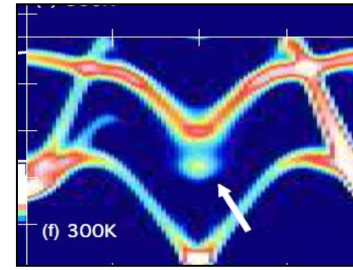
Budai *et al.*
Nature (2014)



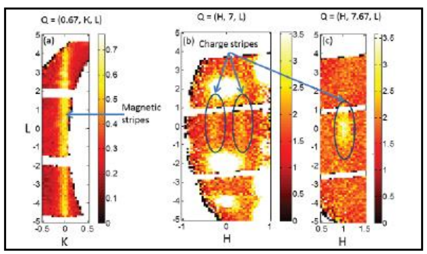
Fuhrman *et al.*
Phys. Rev. Letters (2015)



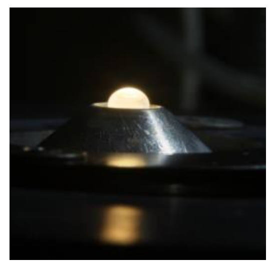
Fitzgibbons *et al.*
Nature Materials (2015)



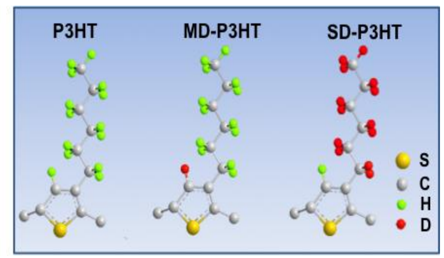
Li *et al.*
Phys. Rev. Letters (2014)



Anissimova *et al.*
Nature Comm. (2014)



Santodonato *et al.*
Nature Comm. (2015)



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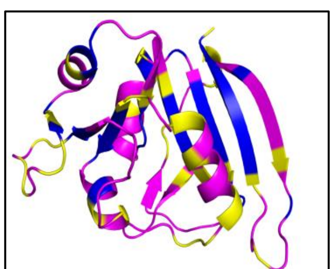
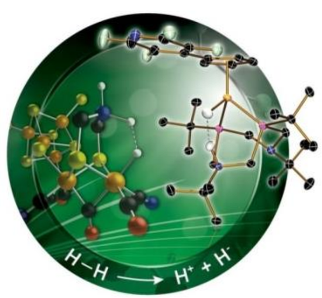
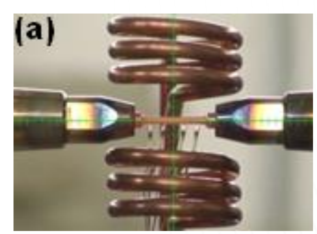


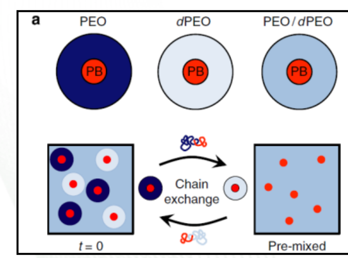
Wan *et al.*
Proc. Nat. Acad of Sci. (2014)



Liu *et al.*
Angew. Chem. Int. Ed. (2014)



Stoica *et al.*
Nature Comm. (2014)



Kelley *et al.*
***Nature Comm.* (2014)**

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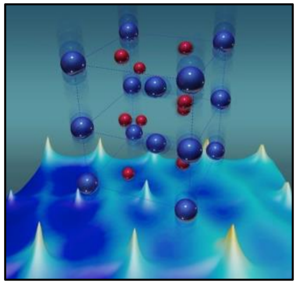
The HFIR and SNS user program is delivering high impact science



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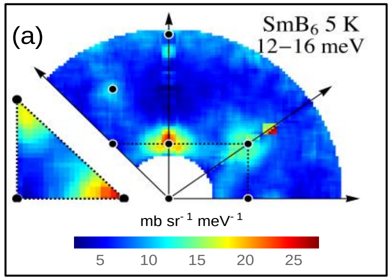

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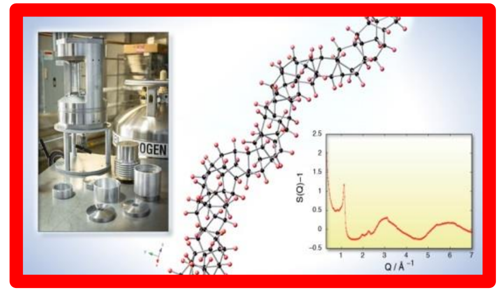

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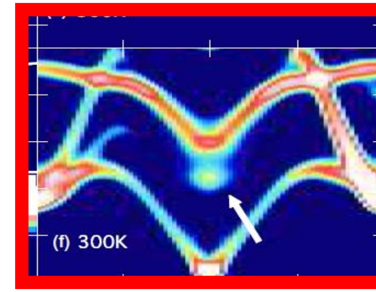

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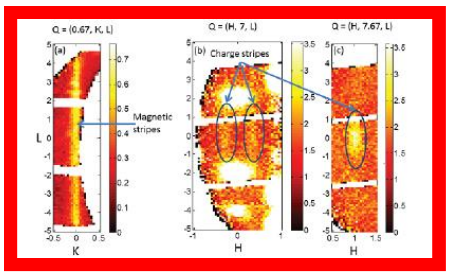

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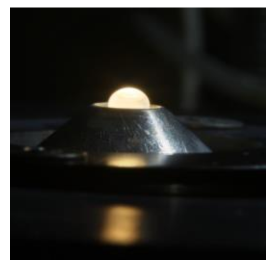

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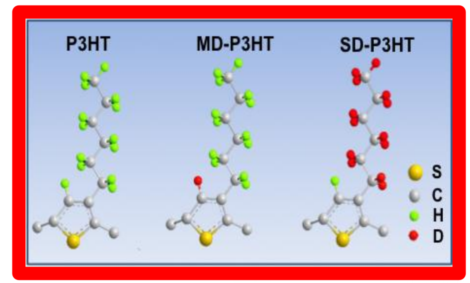

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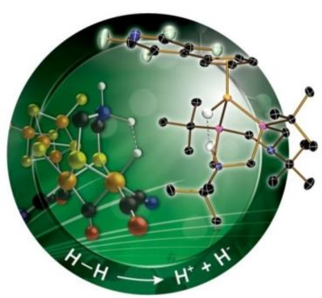

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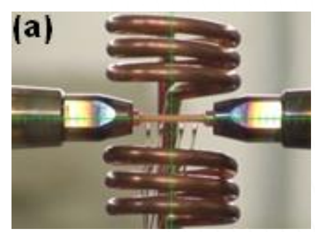

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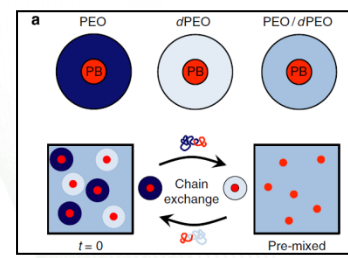
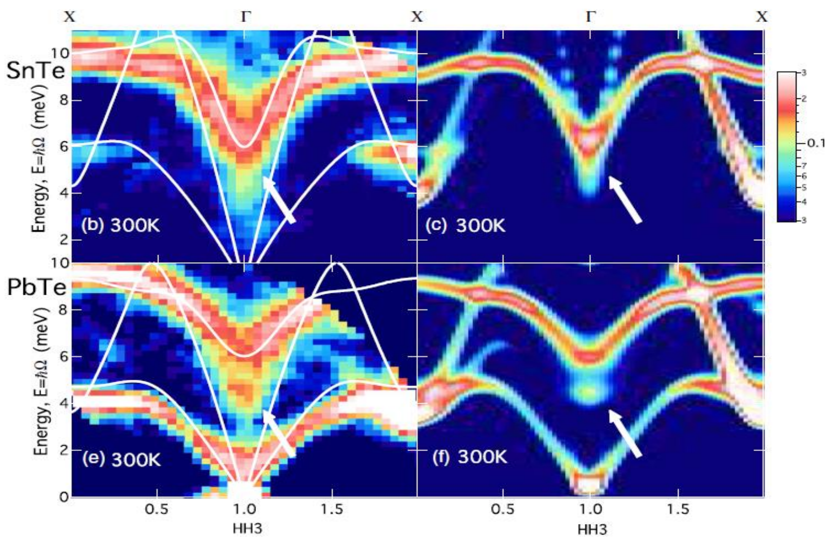
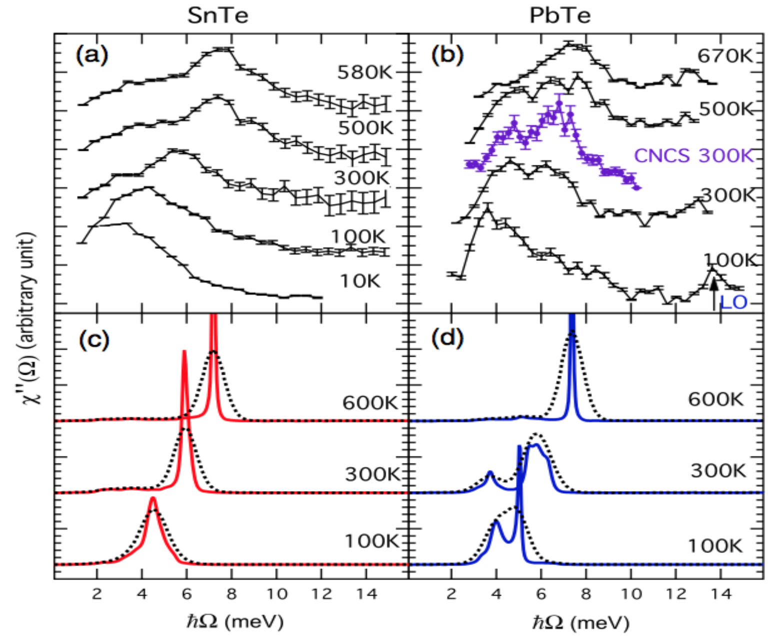


Kelley *et al.*
Nature Comm. (2014)

How thermal conductivity is suppressed in SnTe and PbTe





Significance and Impact

PbTe and SnTe are amongst most efficient thermoelectric materials known. Understanding phonon anharmonicity is important for both fundamental reasons and practical applications, such as improving the efficiency of thermoelectric materials by suppressing their lattice thermal conductivity. This new understanding suggests design of new materials with nested phonon dispersion through doping.

Research Details

The Center for Accelerated Materials Modeling (CAMM) enabled integration of materials modeling/simulation (MD/DFT) directly into the chain for inelastic neutron scattering data analysis (CNCS at SNS and HB3 at HFIR), offline.

C.W. Li, O. Hellman, J. Ma, A.F. May, H.B. Cao, X. Chen, A.D. Christianson, G. Ehlers, D.J. Singh. ***Physical Review Letters***, 175501 (2014). .

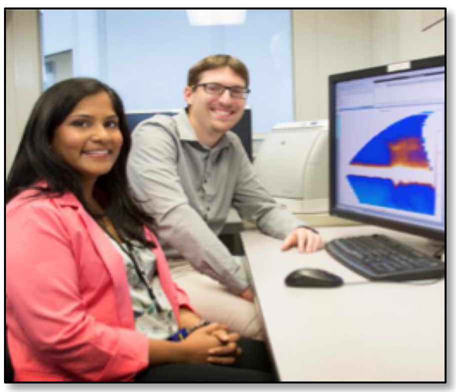
http://camm.ornl.gov for details

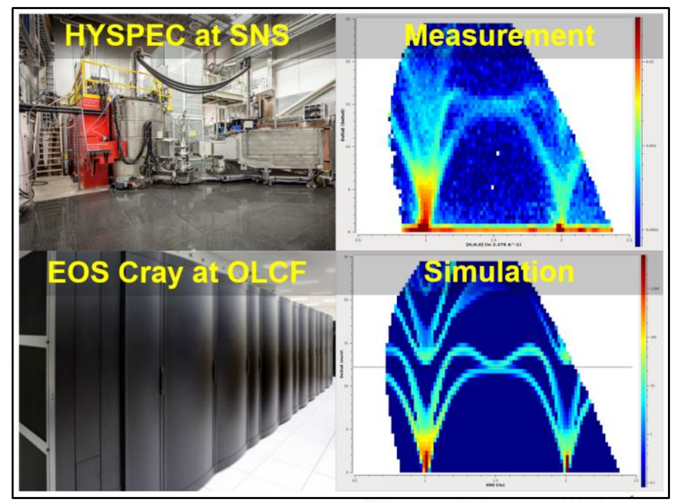
Moving data analysis, modeling and simulation closer to the experiment

Research Details: Ferroelectric instabilities in $SrTiO_3$ (HYSPEC at SNS) using live data streaming. Full scale AIMD simulations (Cray XC30 EOS cluster at OLCF with 11,000 cores) on experiment timescale allowing real time decisions.

Experiment

Data generation → Data acquisition and control → Data reduction (MANTID) → Data analysis and modeling (CAMM)



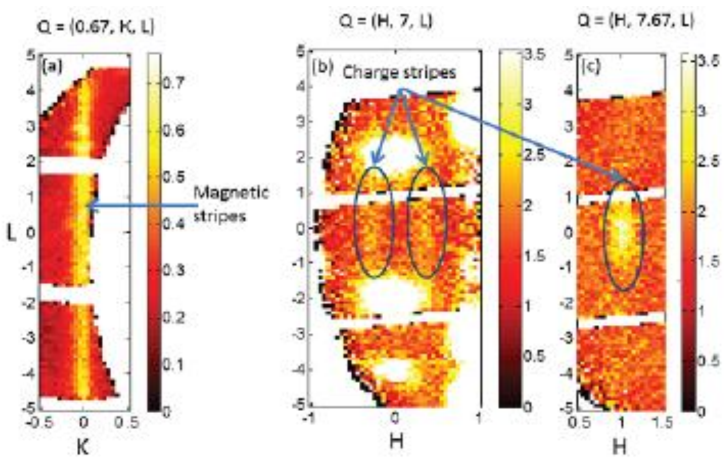


Experiment steering/ feedback

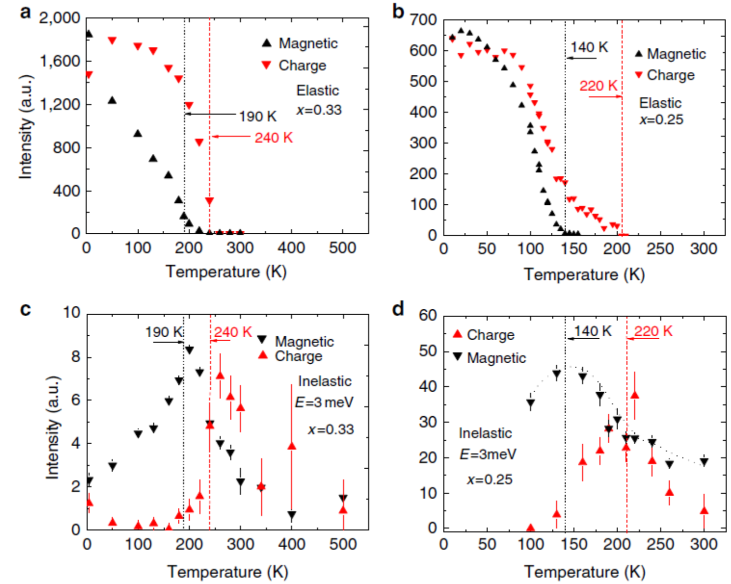
ADARA

Accelerating Data Acquisition, Reduction, and Analysis

First experimental evidence for fluctuating charge-stripes



L-dependence of spin and charge-stripe fluctuations at T = 240 K and E = 5.5 ± 1.5 meV. (a) Magnetic scattering at Q = (0.67, 0, L). (b) Charge stripe fluctuations at Q = (1, 7.67, L), as indicated by ovals.



Significance and Impact

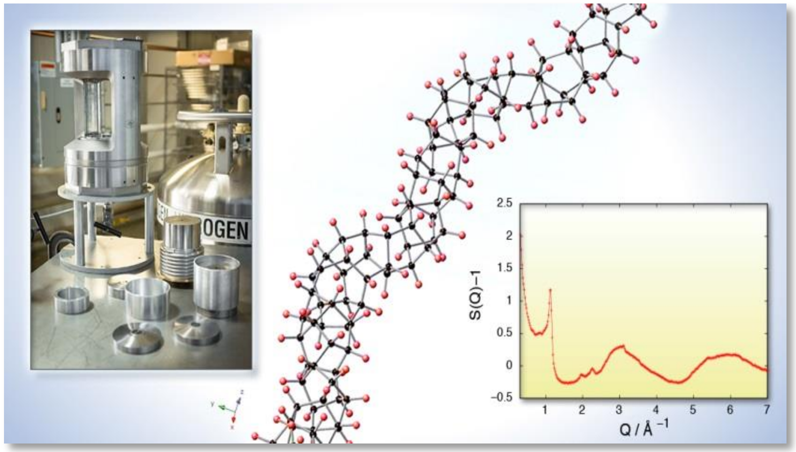
Although there have been theoretic proposals of dynamically fluctuating stripes, evidence has been lacking. The results here open the way towards the quantitative theory of dynamic stripes. Charge-stripe fluctuations may also be present in superconducting cuprates

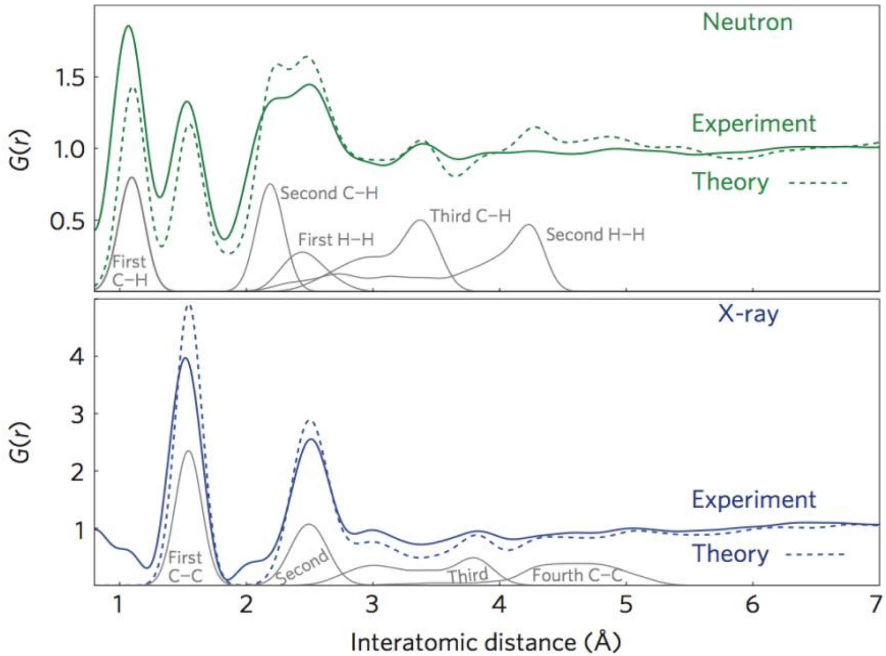
Research Details

Inelastic neutron scattering (ARCS at SNS) was used to detect critical lattice fluctuations, driven by charge-stripe correlations in $La_{2-x}Sr_xNiO_4$.

S. Anissimova, D. Parshall, G. D. Gu, K. Marty, M. D. Lumsden, S. Chi, J. A. Fernandez-Baca, D. L. Abernathy, D. Lamago, J. M. Tranquada, and D. Reznik. ***Nature Communications***. 5 (2014): 3467.

Nanothreads synthesized from benzene are revealed to be diamond-like





Significance and Impact

One of the strongest, stiffest carbon-based nanomaterials with properties that suggest it could have important industrial application in transportation or aerospace manufacturing.

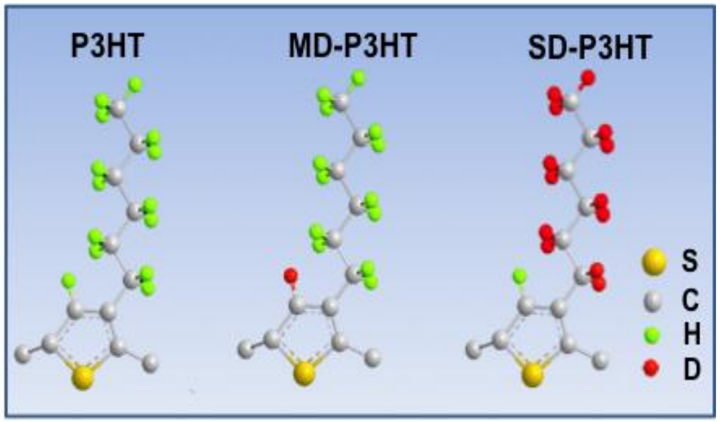
This could by the first member of a whole new class of tuneable nanomaterials.

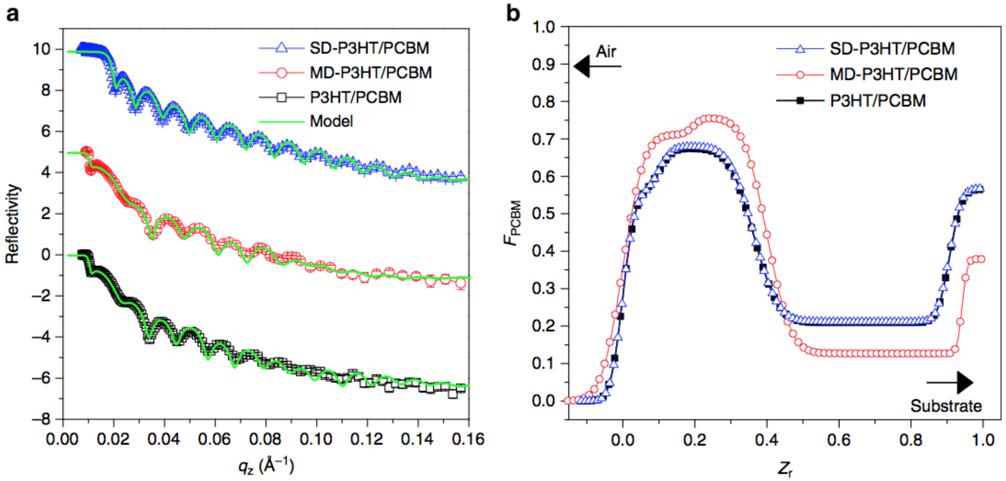
T. C. Fitzgibbons, M. Guthrie, E. Xu, V. H. Crespi, S. K. Davidowski, G. D. Cody, N. Alem, and J. V. Badding, ***Nature Materials***. 43, (2015).

Research Details

20 GPa polymerized benzene at RT (Paris-Edinburgh cell at the SNAP at SNS). X-ray (16IDB and 11IDC at APS) and neutron (NOMAD at SNS) diffraction; Raman spectroscopy; NMR;TEM; DFT for structure optimization. Benzene assembles into *sp*^{3}-bonded, diamond-like chains unlike *sp*^{2}-bonded graphene in conventional high-strength polymers.

Developing a new method for tuning polymers for photovoltaic devices





Significance and Impact

P3HT is an important semiconductor polymer that is mixed with PCBM to fabricate organic photovoltaic devices. Isotopic substitution provides a new means to tune the optoelectronic properties of conducting polymers used for solar cells by affecting their intra- and inter-polymer chain interactions.

M. Shao, J. Keum, J. Chen, Y. He, W. Chen, J.F. Browning, J. Jakowski, B.G. Sumpter, I.N. Ivanov, Y.Z. Ma, C.M. Rouleau, S.C. Smith, D.B. Geohegan, K. Hong and K. Xiao, ***Nature Communications***, **5** 3180 (2014)

Research Details

Center for Nanophase Materials Science (CNMS) researchers used neutron reflectometry (LR at SNS), GIWAXS and GISAXS (8IDE at APS) x-ray scattering, TEM and theoretical modeling were used to show that substitutions D on the backbone or side-chains of conducting polymer poly(3-hexylthiophene)s (P3HT) significantly change their optoelectronic response in P3HT/PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) photovoltaics.

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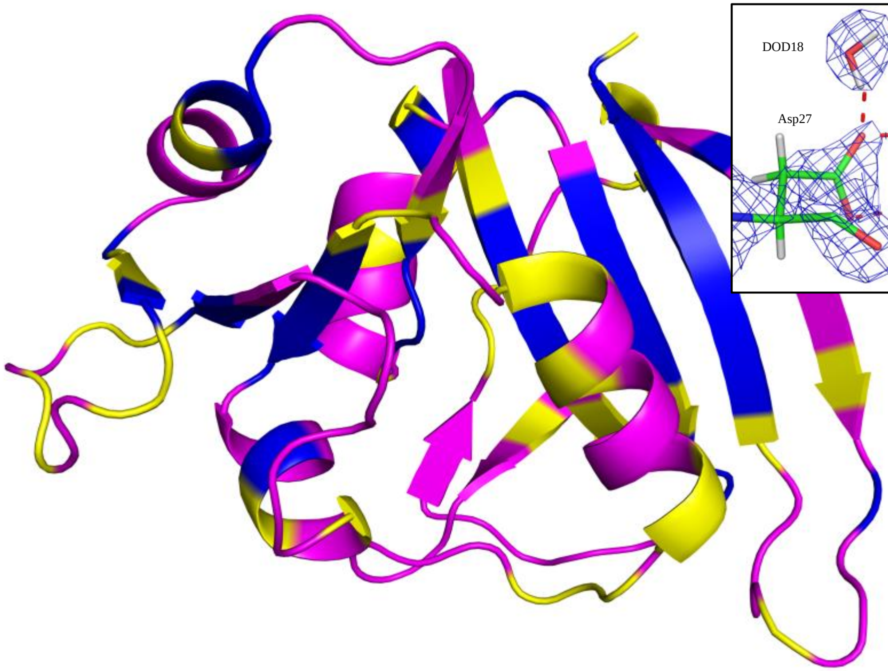
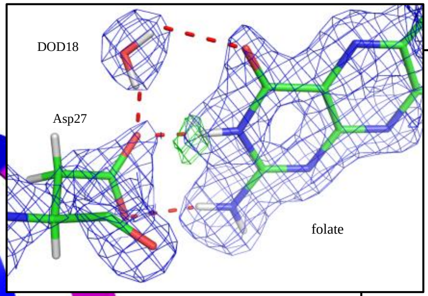
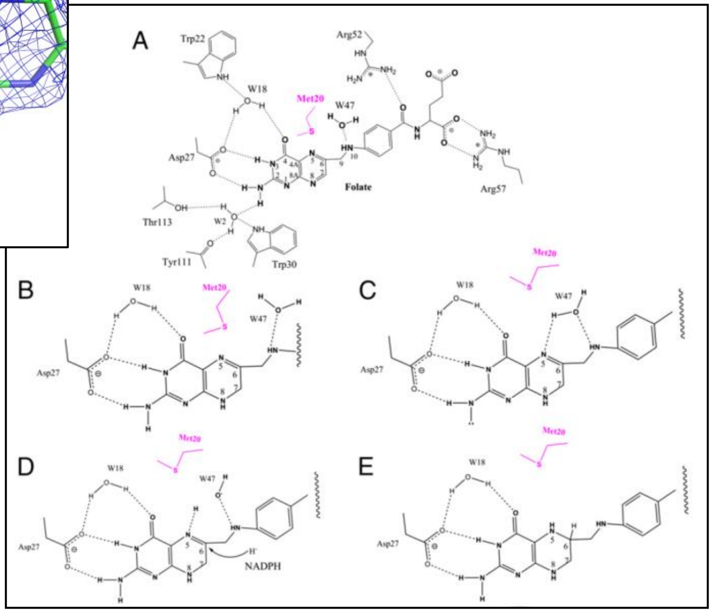
Seeing the chemistry in biology







Significance and Impact

Neutrons can complement X-ray studies with information about the location of H, and therefore reveal the chemistry in biology. DHFR is necessary for nucleotide biosynthesis and a classical drug target. Locatigng H atoms allowed the details of the chemical reaction catalyzed by DHFR to be understood.

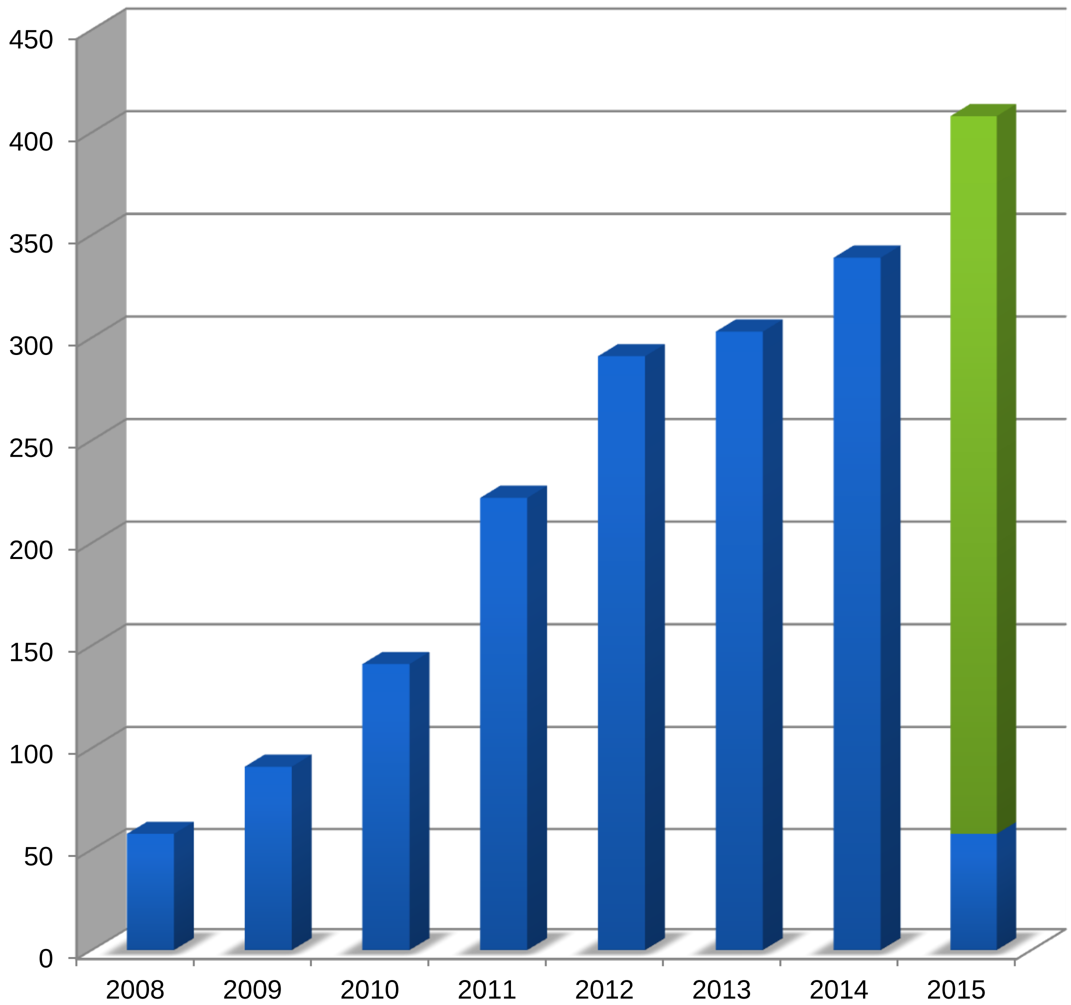
Research Details

First user publication from IMAGINE at HFIR provides the complete details of an enzyme's mechanism (dihydrofolate reductase; DHFR). Neutrons (2.0 Å resolution data) allowed the direct localization of H atoms that were invisible using high resolution X-rays.

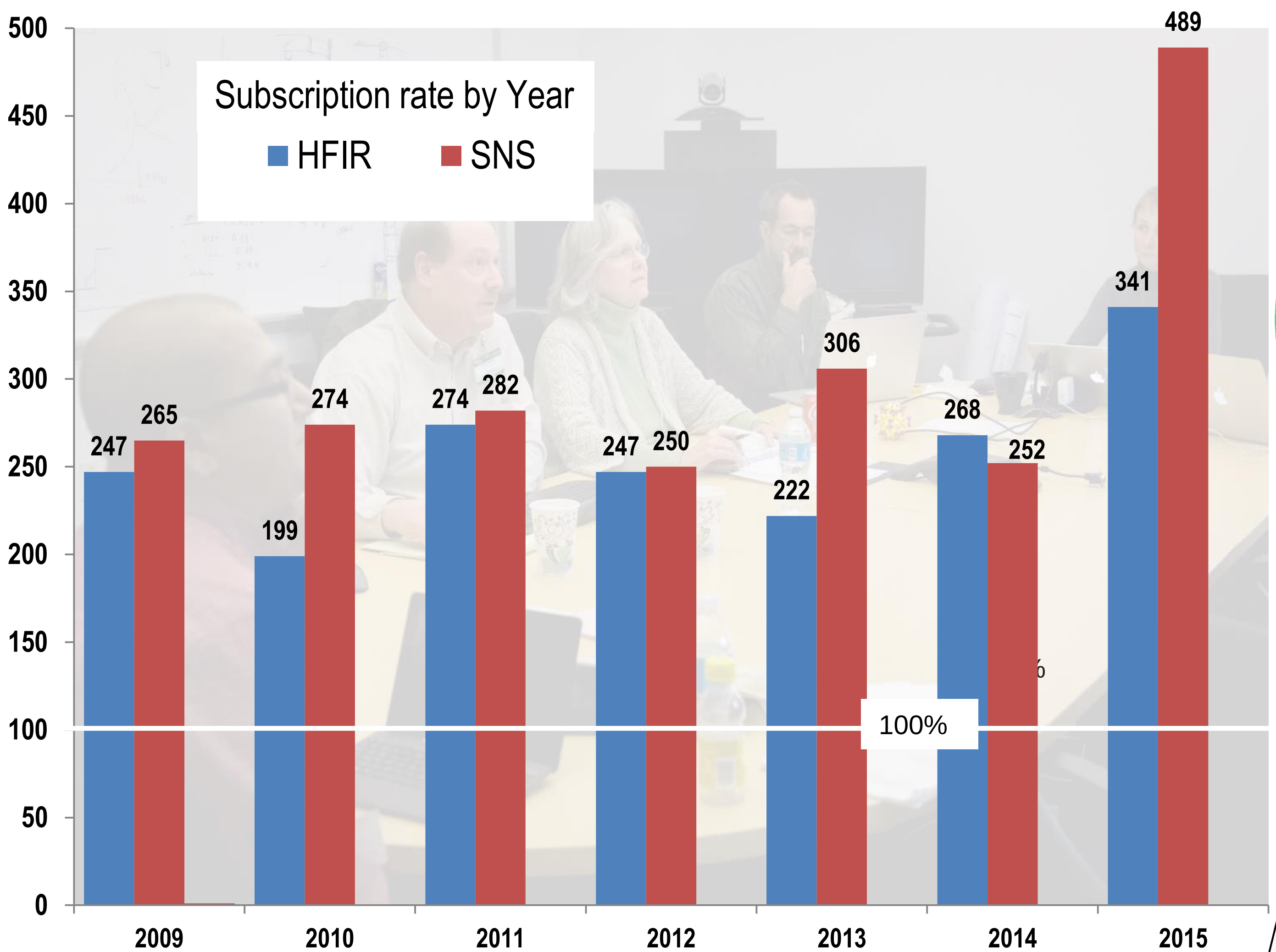
Q. Wan, B. C. Bennett, M. A. Wilson, A. Kovalevsky, P. Langan, E. E. Howell, and C. Dealwis. ***Proceedings of the National Academy of Sciences***. (2014).

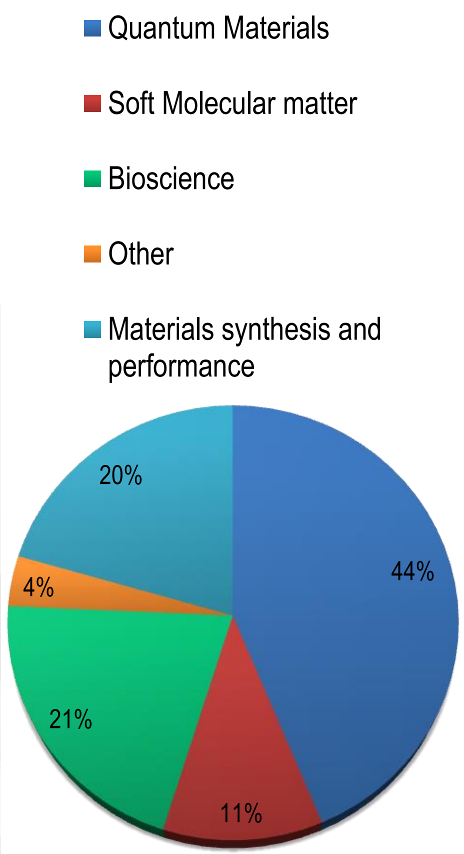
Scientific productivity is on a strong upward trend

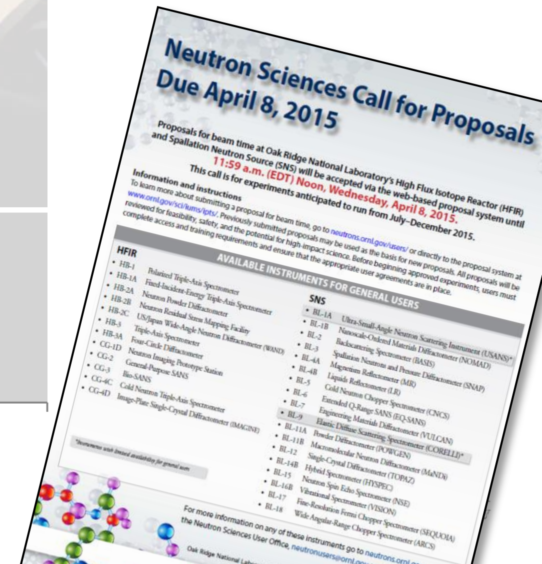
Instrument Publications



All instruments are oversubscribed







Engaging the scientific community to identify emerging science challenges that neutrons can address

Quantum Materials

Quantum Condensed Matter
Lawrence Berkeley National Laboratory
December 2013
Bob Birgeneau

Biosciences

Structural Biology, Bio-materials, and Bioengineering
UC San Diego
January 2014
Susan Taylor

Soft Molecular Matter

Soft Matter
Santa Barbara
May 2014
Fyl Pincus
and Matt Tirrell

Materials Synthesis and Performance

Energy Materials
Chicago
August 2014
George Crabtree
and John Parise

Frontiers in Data Modeling and Simulation Argonne Nat. Lab. March 30-31, 2015
Peter Littlewood

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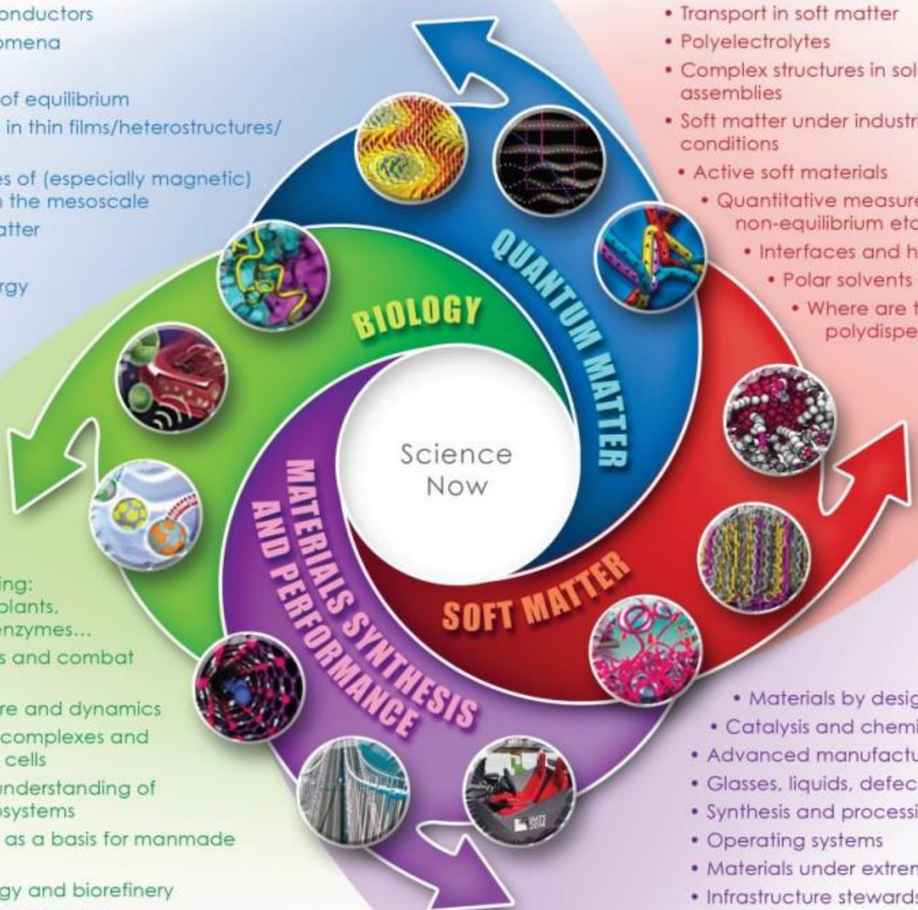
Next Generation Science

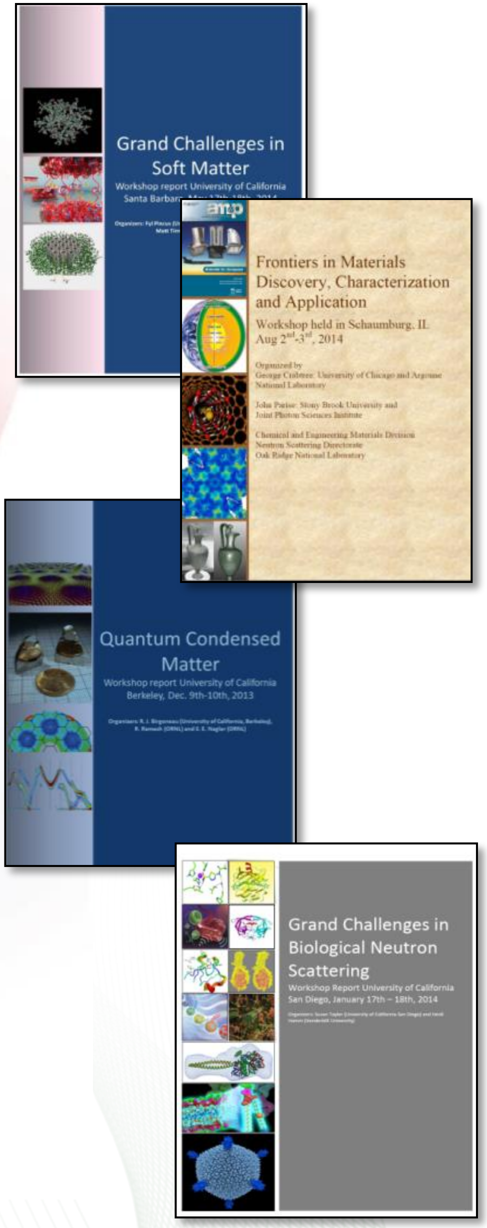
- Exotic ground states in quantum magnets
- Unconventional Superconductors
- Quantum Critical Phenomena
- Itinerant Magnets
- Quantum materials out of equilibrium
- Structure and dynamics in thin films/heterostructures/ nanomaterials
- Spatially resolved probes of (especially magnetic) structure of materials on the mesoscale
- Topological states of matter
- Hydrogen in materials
- Strongly correlated energy materials
- Determining the structure of partially ordered materials including defect structures

- Response of mechanical deformation
- Soft/hard matter composites
- Transport in soft matter
- Polyelectrolytes
- Complex structures in solution/Heirarchical assemblies
- Soft matter under industrial processing conditions
- Active soft materials
  - Quantitative measurements : curvatures, non-equilibrium etc.
    - Interfaces and hybrid systems
      - Polar solvents other than water
        - Where are the effects of polydispersity



- Bioengineering: redesign of plants, organisms, enzymes…
- Design drugs and combat resistance
- Unify structure and dynamics
- Understand complexes and processes in cells
- Integrated understanding of complex biosystems
- Biomaterials as a basis for manmade systems
- Biotechnology and biorefinery
- Understand membranes
- Disorder and flexibility in signaling, communications, regulation
- Kinetics within multi-protein systems

- Materials by design
- Catalysis and chemical reactions
- Advanced manufacturing
- Glasses, liquids, defects and disorder
- Synthesis and processing
- Operating systems
- Materials under extreme conditions
- Infrastructure stewardship
- Future energy and transport
- Porous materials
- Gas absorption
- Pharmaceuticals



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Concepts for next-generation instruments and sources

-being developed and demonstrated through LDRD

Higher flux on sample: Compact moderators; beam optics

Improved detectors: High data rates and resolutions

Polarized beams: Spin nutators and manipulators

Computation: Hierarchy and mesoscale; slow dynamics

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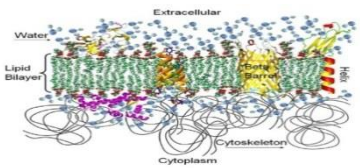
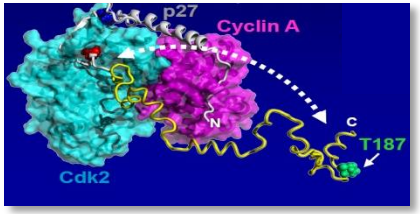
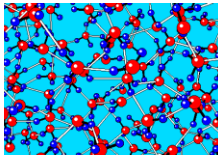
STS can deliver transformative capabilities for complex systems



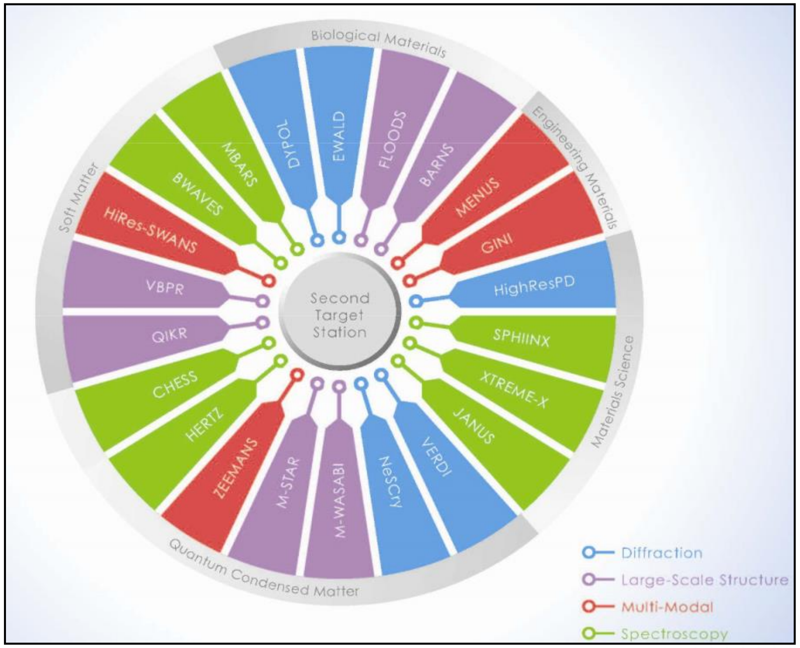
Biological membranes and associated complexes

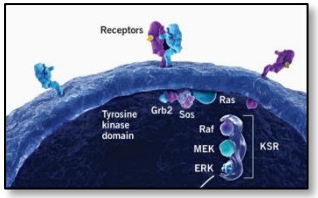


Disorder and flexibility



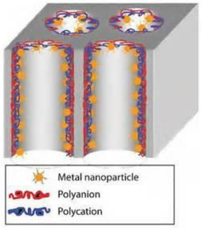
Reactions, catalysis, and kinetics



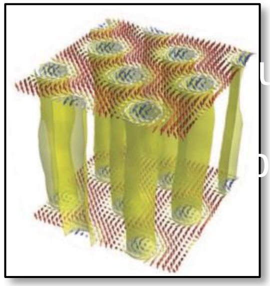


Dynamic functional assemblies

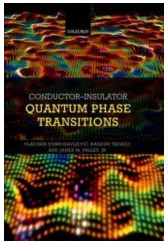
Novel manufacturing and processing



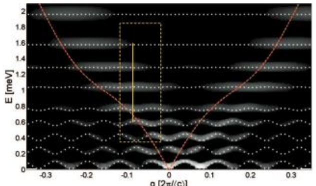
Hierarchical materials



Topological materials and excitations



Extreme conditions and new phases of matter



Artificial crystals and heterostructures

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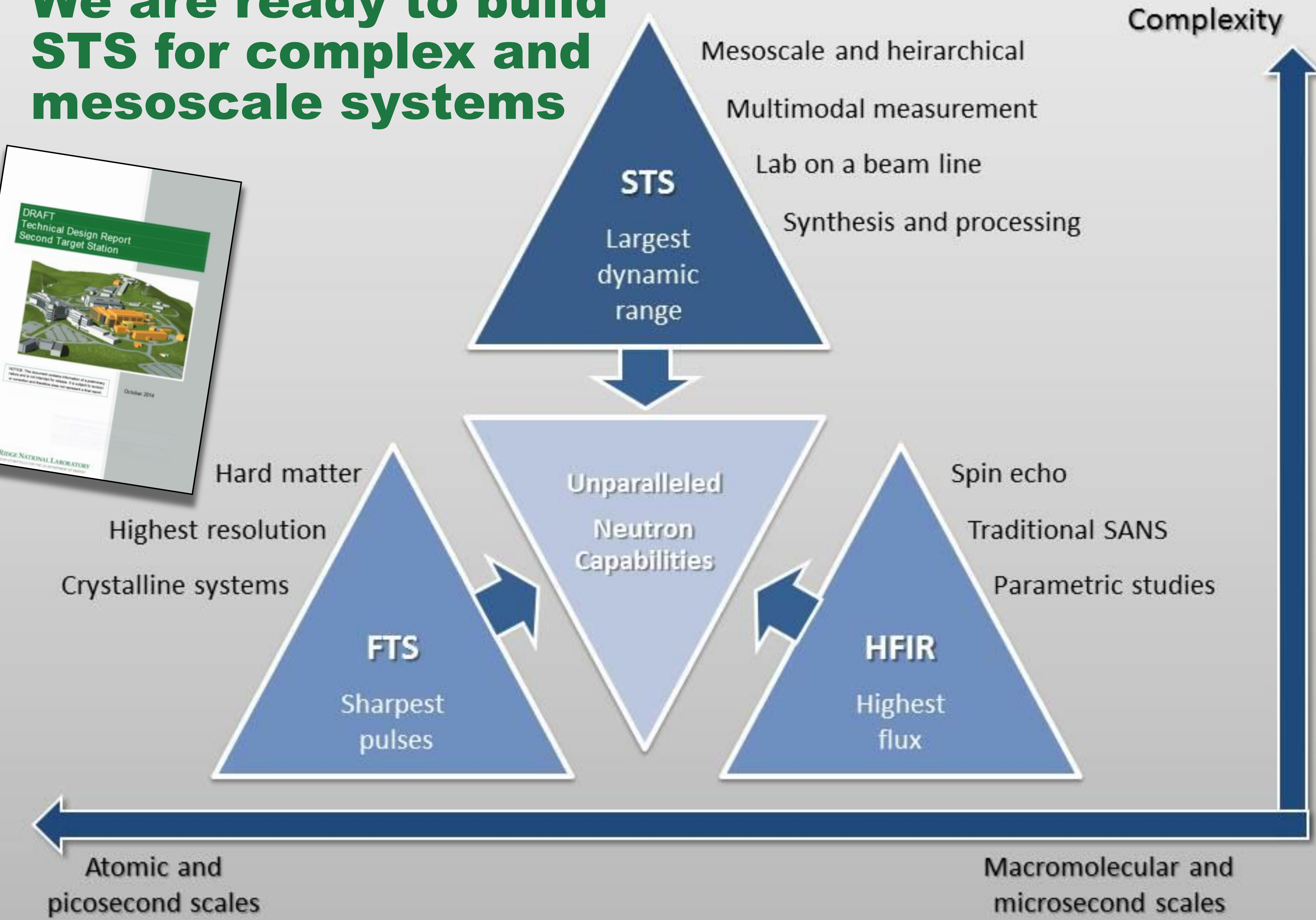
We are ready to build STS for complex and mesoscale systems



Best neutron capabilities for researchers to address the most important emerging challenges

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

- Facility improvement
- New technologies and methods for next generation science
- Integration with computational methods and other exp. techniques

Long-term plan

Second target station at SNS to double neutron science capacity and expand capabilities by 2-3 orders of magnitude, new capabilities for complexity

- Optimize science across complementary sources
- Positioning to address the emerging grand challenges of our sponsors and research community

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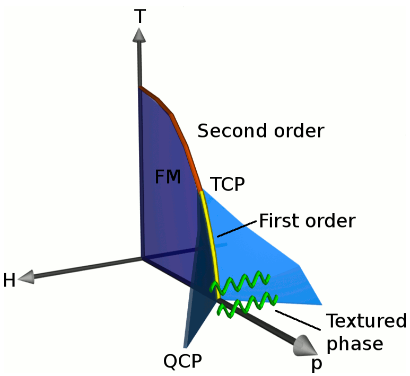
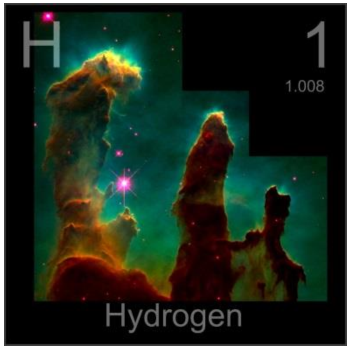
Summary

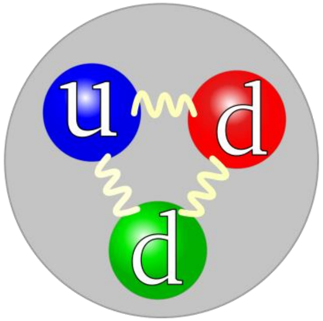
- HFIR and SNS are producing high impact science
- Scientific productivity is on a strong upward trend
- The user community is being engaged to look to the future and define the emerging grand challenges
- We are responding to those challenges by developing new concepts and technologies for next generation instruments and sources.
- Our short term focus is on maximizing the capabilities of the SNS and HFIR
- Our long term focus is on building a second target station at the SNS
- We aim to provide the best possible neutron capabilities for researchers to use to address the biggest and most important problems

Additional Material

Why neutrons are unique







Measure dynamics and structure

High contrast to light elements

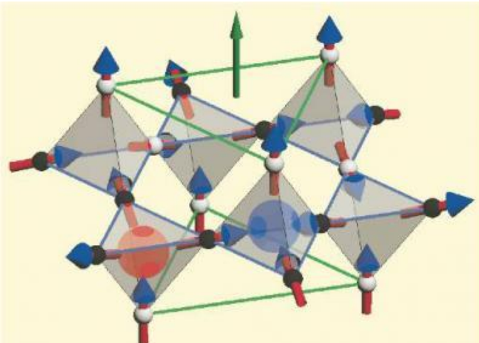
High penetrability

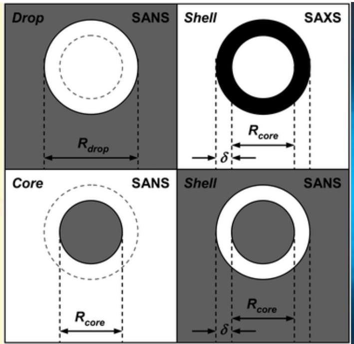
Fundamental particle

Sensitivity to magnetism

Isotope substitution

Direct connection to theory and simulation





World's most intense pulsed, accelerator-based neutron source

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Backscattering Spectrometer (BASIS) • BL-2
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Eugene Mamontov • 865.574-5109 • mamontove@ornl.gov

Nanoscale-Ordered Materials Diffractometer (NOMAD) • BL-1B
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuefeind • 865.241.1635 • neuefeindjc@ornl.gov

Wide Angular-Range Chopper Spectrometer (ARCS) • BL-18
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Doug Abernathy • 865.617.5624 • abernathydl@ornl.gov

Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) • BL-17
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Matthew Stone • 865.202.6898 • stonemb@ornl.gov

Ultra-Small-Angle Neutron Scattering Instrument (USANS) • BL-1A (2014*)
Life sciences, polymers, materials science, earth and environmental sciences
Michael Agamalian • 865.382.6367 • magamalian@ornl.gov

Vibrational Spectrometer (VISION) • BL-16B
Vibrational dynamics in molecular systems, chemistry
Yongqiang Cheng • 865.5576.9064 • chengy@ornl.gov

BL-16A

Spallation Neutrons and Pressure Diffractometer (SNAP) • BL-3
Materials science, geology, earth and environmental sciences
Chris Tulk • 865.574.5764 • tulkca@ornl.gov

Neutron Spin Echo Spectrometer (NSE) • BL-15
High-resolution dynamics of slow processes, polymers, biological macromolecules
Michael Ohl • 865.574.8426 • ohlme@ornl.gov

Hybrid Spectrometer (HYSPEC) • BL-14B
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Barry Winn • 865.805.6819 • winnbl@ornl.gov

BL-14A

Magnetism Reflectometer • BL-4A
Chemistry, magnetism of layered systems and interfaces
Valeria Lauter • 865.387.5389 • lauterv@ornl.gov

Liquids Reflectometer • BL-4B
Interfaces in complex fluids, polymers, chemistry
John Ankner • 865.377.4523 • anknerjf@ornl.gov

Fundamental Neutron Physics Beam Line • BL-13
Fundamental properties of neutrons
Geoffrey Greene • 865.576.0023 • greenegl@ornl.gov

Cold Neutron Chopper Spectrometer (CNCS) • BL-5
Condensed matter physics, materials science, chemistry, biology, environmental science
Georg Ehlers • 865.206.0824 • ehlersg@ornl.gov

Macromolecular Neutron Diffractometer (MaNDi) • BL-11B
Atomic-level structures of membrane proteins, drug complexes, DNA
Leighton Coates • 865.964-8651 • coatesl@ornl.gov

Single-Crystal Diffractometer (TOPAZ) • BL-12
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
Christina Hoffmann • 865.576.5127 • choffmann@ornl.gov

BL-8A

BL-8B

Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) • BL-6
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
William Heller • 865.241.0093 • hellerwt@ornl.gov

Elastic Diffuse Scattering Spectrometer (CORELLI) • BL-9 (2014*)
Detailed studies of disorder in crystalline materials
Feng Ye • 865.576.0931 • yef1@ornl.gov

Versatile Neutron Imaging Instrument at SNS (VENUS) • BL-10
Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology
Hassina Bilheux • 865.384.9630 • bilheuxhn@ornl.gov

Powder Diffractometer (POWGEN) • BL-11A
Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures
Ashfia Huq • 630.986.7321 • huqa@ornl.gov

Engineering Materials Diffractometer (VULCAN) • BL-7
Mechanical behaviors, materials science, materials processing
Ke An • 865.919.5226 • kean@ornl.gov

*Scheduled commissioning date

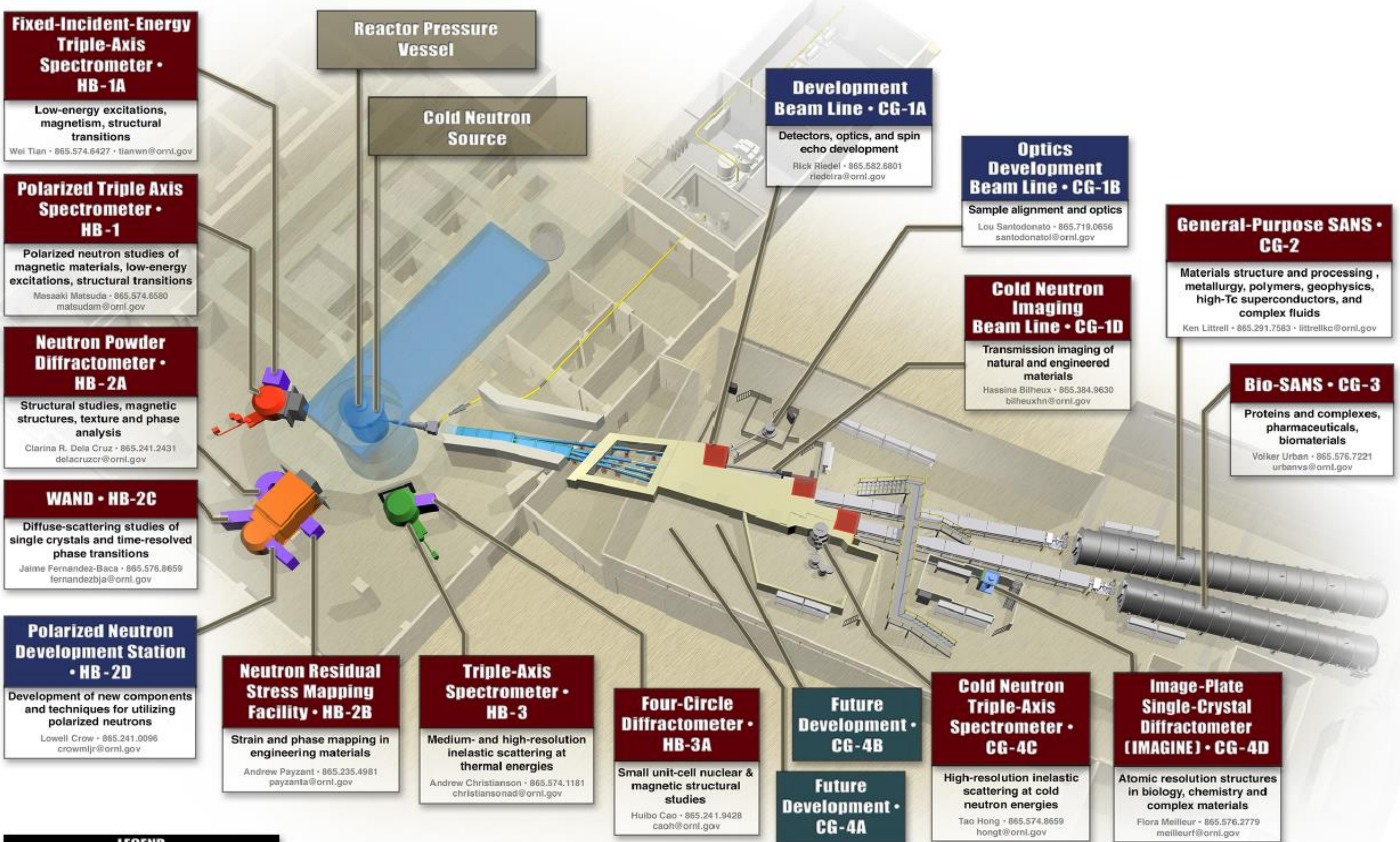
LEGEND
- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

The Spallation Neutron Source is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

14-G00875/gim

High Flux Isotope Reactor at Oak Ridge National Laboratory

The United States' highest flux reactor-based neutron source



LEGEND

- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

07-G00244N/gim

U.S. DEPARTMENT OF ENERGY Office of Science

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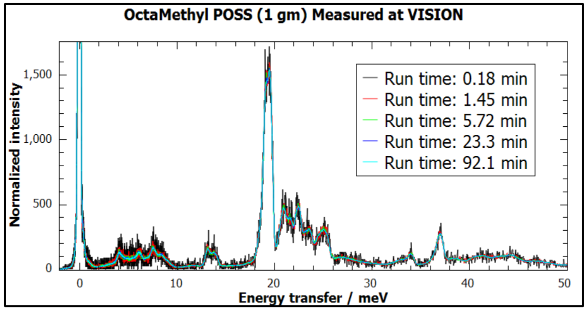
Neutron Sciences

Programmatic investments are producing new science opportunities

New instruments coming on-line

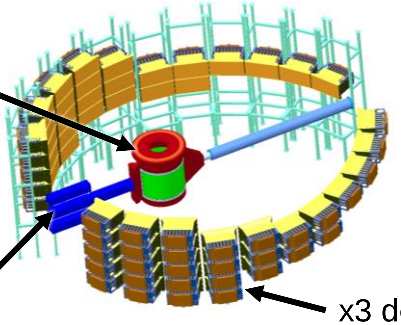
VISION and MaNDi in User program.
CORELLI and USANS commissioning.

High throughput data from VISION



Planned instrument upgrades

Efficiency improvements in SNS powder diffraction instruments.



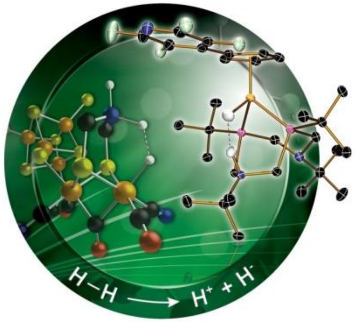
Powgen upgrade

Investments in science capabilities for studying magnetism

- Growing high magnetic field capabilities
- Polarized beam analysis on HYSPEC
- Spin-encoded methods for high resolution

Anger camera development delivering science on TOPAZ and MaNDi

Neutron diffraction on TOPAZ reveals the process of heterolytic cleavage of H_2 in hydrogenase enzymes



Liu et al., *Angew. Chem. Int. Ed.* (2014)

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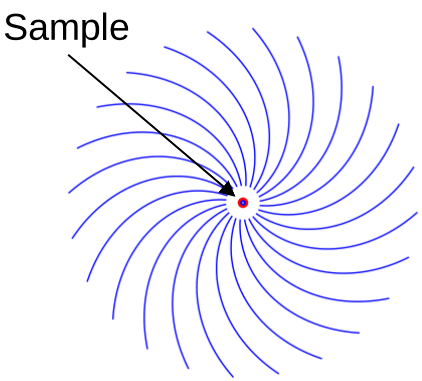
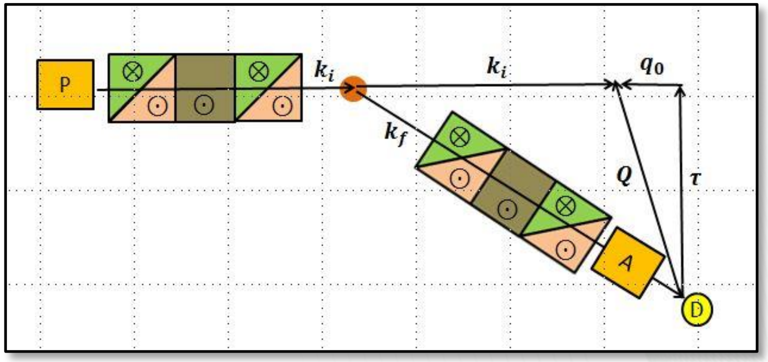
FY15: Directed LDRD

Next Generation Neutron Source and Instrumentation

	Description	FY15 $k
LOIS 7465	Volume-Moderator Demonstration Facility	$475.3
LOIS 7406	High-Resolution Solid State Detectors	$480.0
LOIS 7374	Development of Resonance Spin-Echo Techniques	$363.4
LOIS 7331	Development of Wide Angle Velocity Selector (WAVES)	$481.3
	Total	$1,800.0



WAVES concept



Resonant spin echo using Wollaston prisms

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FY15–Establishing the STS science case

3 "heroic" experiments/developments

	Description	Strategic Objective	Current Budget Request		
			FY15	FY16	FY17
LOIS 7637	Spectroscopy at Extreme High Pressures	Establish SNS as international leader in high-P neutron spectroscopy – STS instruments: CHESS, XTREME-X	\$699.2k	\$657.4k	\$140k
LOIS 7640	Dynamic Nuclear Polarization	Develop and demonstrate DNP – deliver >1000-fold gain in diffraction capability for proteins – STS instrument: DYPOL	\$992k	\$2,713k	\$89k
LOIS 7641	High-Resolution Small/Wide Angle Neutron Scattering	Develop a test instrument and demonstrate simultaneous atomic through molecular-scale structural evolution in hierarchical materials – STS instrument: HiRes-SWANS	\$472k	\$777k	\$124k
		Total	\$2,163.2k	\$4,147.4k	\$353k

Complementarity across 3 ORNL neutron sources provides opportunity for instrument optimization

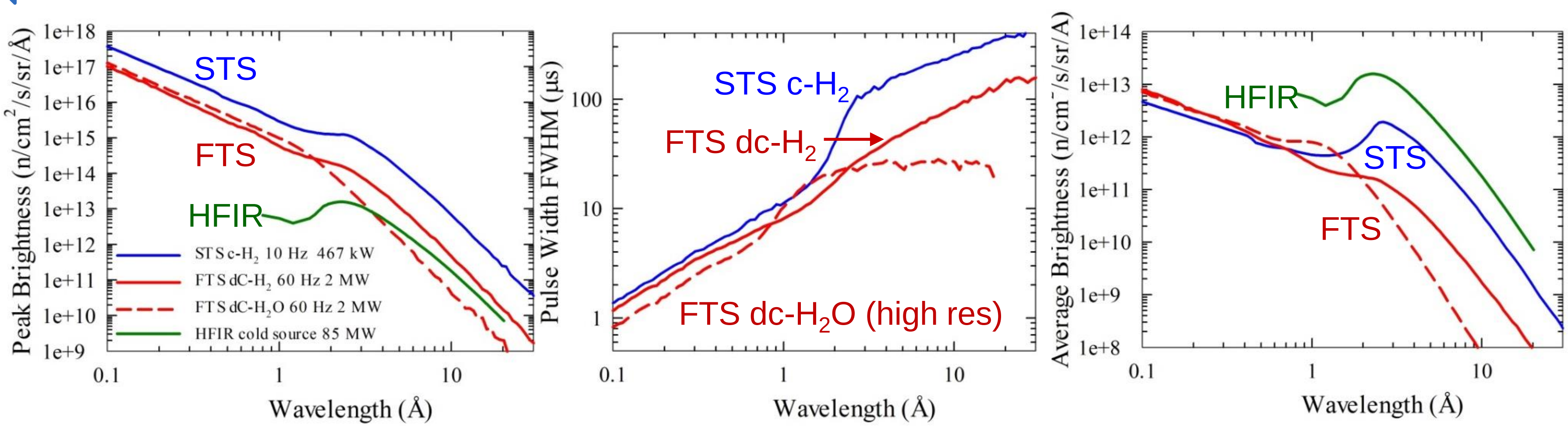
STS: Optimized for cold neutrons with high peak brightness

(Coupled moderators, 10 Hz)

FTS: Optimized for high-wavelength resolution across neutron spectrum

(Decoupled moderators, 60 Hz)

HFIR: Optimized for cold and thermal neutrons with high time-averaged brightness



TDR activities, FY 2014

Core team of engaged individuals

Establish initial design concepts

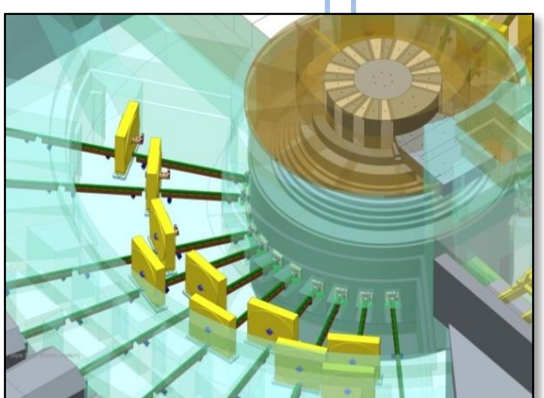
- Plan for instrument suite
- 3 moderators (FY13 LDRD)
- Compact tungsten target
- Proton beamline lattice to STS

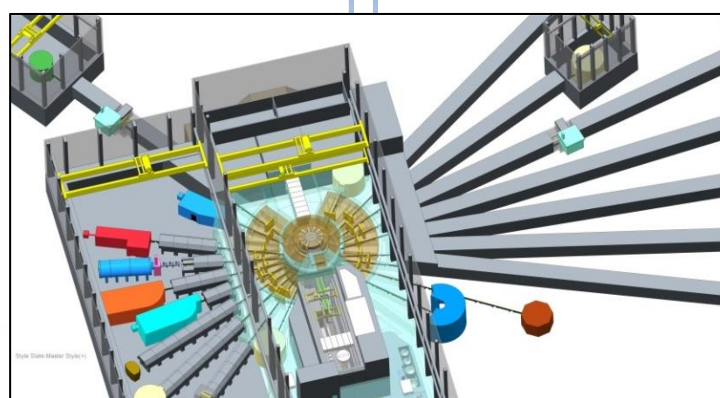
Define Work Breakdown Structure to level 3

- Major subsystems (e.g., individual instruments, accelerator RF systems)
- Top-down cost estimates

Engage A/E for site layout and definition of conventional facilities

- ORNL estimators will generate initial cost estimate





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