ORNL/Georgia Tech Joint Workshop in Neutron Science and Scattering

Date: Wednesday, January 27, 2016

Organizing Committee: Nazanin Bassiri-Gharb, Julia Kubanek, Kathryn Bond, Greg Smith, Gabrielle Boudreau

Objective: Establish stronger links between ORNL Neutron Sciences Directorate and Science and Engineering Researchers at Georgia Tech.

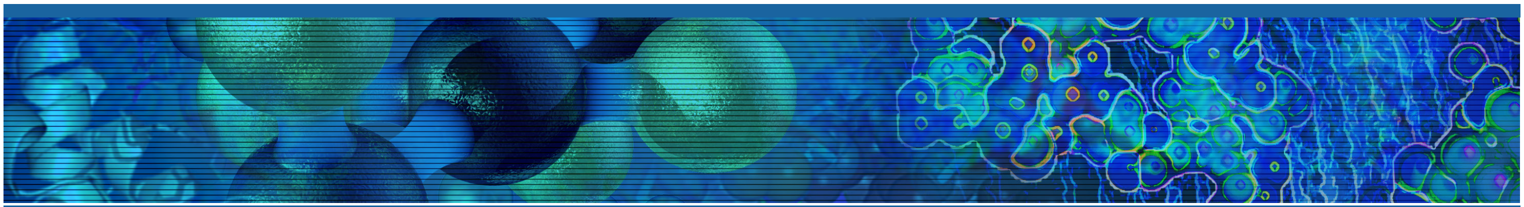
Location: Georgia Institute of Technology
Marcus Nanotechnology Building, Room 1117/1118
345 Ferst Drive NW, Atlanta, GA 30318

Schedule:

8:00 – 8:30	**Continental Breakfast, Registration**
8:30 – 8:40	**Welcome by Steve Cross** Executive Vice President for Research Georgia Institute of Technology
8:40 – 9:00	**Welcome by Alan Tennant** Chief Scientist, Neutron Sciences Oak Ridge National Laboratory
9:00 – 9:25	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Study of Hydrogen Bonding in Energy Materials Using Single Crystal Neutron Diffraction* Xiaoping Wang, Chemical and Engineering Materials Division
9:25 – 9:50	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Thin Films and Interfaces* Mike Fitzsimmons, Quantum Condensed Matter Division
9:50 – 10:15	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Universal Characteristics of Water Dynamics in Restricted Geometries Using Quasi-elastic Neutron Scattering* Souleymane Omar Diallo, Chemical and Engineering Materials Division

10:15 – 10:45	**Coffee Break**
10:45 – 10:57	**CoE speaker (10 minute presentation + 2 minute discussion)** *Process-structure-property relations in polymer organic electronics* Martha Grover, School of Chemical & Biomolecular Engineering
10:57 – 11:09	**CoS speaker (10 minute presentation + 2 minute discussion)** *Organic-inorganic Materials Systems for Energy Applications* Mark Losego, School of Materials Science and Engineering
11:09 – 11:21	**CoE speaker (10 minute presentation + 2 minute discussion)** *Understanding Atomic Vibrations in Disordered Materials* Asegun Henry, Woodruff School of Mechanical Engineering
11:21 – 11:33	**CoS speaker (10 minute presentation + 2 minute discussion)** *Biochemical and Structural Characterization of Unusual Hydrolytic Enzymes* Raquel Lieberman, School of Chemistry & Biochemistry
11:33 – 11:45	**CoE speaker (10 minute presentation + 2 minute discussion)** *Pathways to Improved Lifetime of Electrochemical Systems: Understanding Dynamic Materials Processes* Matt McDowell, Woodruff School of Mechanical Engineering
11:45 – 12:15	**Discussion of Future Opportunities for Collaborative Research**
12:15 – 1:45	**Lunch and Poster Session**
1:45 – 2:10	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Macromolecular Neutron Crystallography: Elusive Species Protonation States and Proton Transfer* Andrey Kovalevsky, Biology and Soft Matter Division
2:10 – 2:35	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Bio-Materials and Scattering* William Heller, Biology and Soft Matter Division
2:35 – 3:00	**ORNL Presentation (20 minute presentation + 5 minute discussion)** *Soft Matter: Micelle Aggregation and Labelling* Changwoo Do, Biology and Soft Matter Division
3:00 – 3:30	**Coffee Break**
3:30 – 3:42	**CoS speaker (10 minute presentation + 2 minute discussion)** *Synthesis, Structure and Reaction Chemistry of Hydride-Bridged Coinage*

	Metal Complexes Joseph Sadighi, School of Chemistry & Biochemistry
3:42 – 3:54	**CoE speaker (10 minute presentation + 2 minute discussion)** *Neutron Spectroscopy on Quantum Materials* Martin Mourigal, School of Physics
3:54 – 4:06	**CoS speaker (10 minute presentation + 2 minute discussion)** *Exploring the Multiscale Physics of Muscle Through Small-angle X-ray Scattering* Simon Sponberg, School of Physics and School of Applied Physiology
4:06 – 4:18	**CoE speaker (10 minute presentation + 2 minute discussion)** *Multiscale Electron Microscopy for Characterization of Materials in Extreme Environments* Josh Kacher, School of Materials Science & Engineering
4:18 – 4:30	**CoS speaker (10 minute presentation + 2 minute discussion)** *Engineering Functional Protein Nanoparticles* M.G. Finn, School of Chemistry & Biochemistry and School of Biology
4:30 – 5:00	**Discussion of Future Opportunities for Collaborative Research** All participants



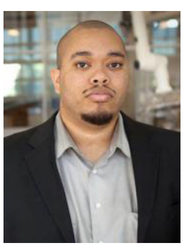
ORNL/Georgia Tech Joint Workshop in Neutron Science and Scattering

January 27, 2016

Georgia Institute of Technology Presenters' Biographies

M.G. Finn, mgfinn@gatech.edu
Dr. M.G. Finn is Chair of the School of Chemistry and Biochemistry at Georgia Tech, and Director of the Center for Pediatric Nanomedicine. Finn studied chemistry at Caltech and earned his Ph.D. at MIT. Following a postdoctoral fellowship at Stanford, he served on the faculties of the University of Virginia and The Scripps Research Institute, moving to Georgia Tech in 2013. Finn's current interests include the use of virus particles as molecular and catalytic building blocks for biomedical science and functional materials development. He is Editor-in-Chief of the journal ACS Combinatorial Science.

Martha Grover, martha.grover@chbe.gatech.edu
Dr. Grover is an associate professor of Chemical & Biomolecular Engineering at Georgia Tech. Her research activities in process systems engineering focus on understanding macromolecular organization and the emergence of biological function. The Grover group is dedicated to the development of tractable and practical approaches for the engineering of macroscale behavior via explicit consideration of molecular and atomic scale interactions. They focus on applications involving the kinetics of self-assembly, specifically those in which methods from non-equilibrium statistical mechanics do not provide closed form solutions. General approaches employed include stochastic modeling, model reduction, machine learning, experimental design, robust parameter design, and estimation.



Asegun Henry, asegun.henry@me.gatech.edu
Dr. Asegun Henry is an Assistant Professor in the George W. Woodruff School of Mechanical Engineering at Georgia Tech. He received his Ph.D. from MIT in 2009 under the supervision of Professor Gang Chen. He also holds a B.S. in mechanical engineering from Florida A & M University and an M.S. in mechanical engineering from MIT. Dr. Henry's primary research background is in heat transfer, with a specific emphasis on understanding energy transport storage and conversion at the atomic level. Prior to joining Georgia Tech, Asegun also worked as a postdoc in the materials theory group at Oak Ridge National Laboratory (ORNL) developing an approach to predict the thermal conductivity of materials fully from first principles, and as a postdoc in the materials science department at Northwestern University, where he studied the thermodynamic properties of reactive oxides for use in high temperature solar thermochemical reactors. After Northwestern, Asegun worked as a fellow in the advanced research projects agency – energy (ARPA-E), where he focused on identifying new program areas, such as higher efficiency, lower cost solar and thermal energy conversion and storage. www.ase.gatech.edu

Josh Kacher, josh.kacher@mse.gatech.edu
Dr. Kacher is an assistant professor of Materials Science and Engineering at Georgia Institute of Technology. His primary research interests are in understanding the mechanical behavior of materials in extreme environments using in situ electron microscopy techniques. His research group is interested in understanding the mechanical behavior of materials in extreme environments. This includes understanding how environmental factors such as irradiation or liquid metal embrittlement affect the mechanical properties and failure modes of materials. He received his PhD from the University of Illinois working with Ian Robertson and completed a post doc at Berkeley working with Andrew Minor.

Oak Ridge National Laboratory

Georgia Institute of Technology®

ORNL/Georgia Tech Joint Workshop in Neutron Science and Scattering

Raquel Lieberman, raquel.lieberman@chemistry.gatech.edu

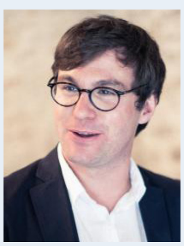
Dr. Raquel Lieberman is an Associate Professor in the School of Chemistry & Biochemistry at Georgia Institute of Technology. Dr. Lieberman joined the faculty in January 2008 after conducting postdoctoral work with Greg Petsko at Brandeis and earning her PhD with Amy Rosenzweig at Northwestern. Her research group focuses on protein structure and function, particularly misfolding as well as hydrolysis that occurs within or near the lipid membrane, using structural, biophysical, and biochemical approaches.

Mark Losego, losego@gatech.edu

Dr. Losego is an Assistant Professor of Materials Science and Engineering at Georgia Tech. His research group explores materials systems that interface organic and inorganic constituents for a wide range of applications including solar fuels, capacitive energy storage, waste heat recovery, and technical textiles. Combining expertise in vacuum processing equipment design, construction, and operation (e.g., ALD, MLD, PVD, etc.) with chemical solution synthesis methods, the Losego group seeks to obtain precise control over interfacial structure to elucidate the origin of fundamental transport properties of relevance to organic-inorganic hybrid device performance.

Matthew McDowell, mattmcdowell@gatech.edu

Dr. Matthew McDowell joined Georgia Tech in the fall of 2015 as an assistant professor with a joint appointment in the George W. Woodruff School of Mechanical Engineering and the School of Materials Science and Engineering. He received his Ph.D. in 2013 from the Department of Materials Science and Engineering at Stanford University and subsequently was a postdoc at Caltech. His research group's work encompasses both the fundamental investigation of materials transformations in electrochemical systems, as well as the development of improved energy systems through materials and device engineering.



Martin Mourigal, mourigal@gatech.edu

Dr. Mourigal joined Georgia Tech in 2015 as an assistant professor in the School of Physics. Prior to joining Georgia Tech, he completed a three-year postdoctoral research fellowship at the Institute for Quantum Matter at Johns Hopkins University in Baltimore, Maryland. He earned his PhD in experimental physics jointly from the Institut Laue-Langevin in Grenoble, France and École Polytechnique Fédérale de Lausanne in Lausanne, Switzerland. His research interests combine materials characterization, neutron scattering, data analysis and theory to explore novel magnetic and electronic states of quantum matter.

Joseph Sadighi, joseph.sadighi@chemistry.gatech.edu

Dr. Sadighi is currently an Associate Professor in the School of Chemistry and Biochemistry at Georgia Tech. He studied chemistry at Williams College, earned his Ph.D. from MIT, and held a postdoctoral position at Caltech before beginning his independent career. Research in the Sadighi group focuses on the development of low-coordinate complexes of late transition metals, particularly the group 11 metals, featuring unusual metal-metal and metal-element bonding. These bonding motifs are sought to enable difficult bond-forming and bond-breaking processes, and thus lead to new catalytic small molecule transformations.

Simon Sponberg, simon.sponberg@physics.gatech.edu

Simon Sponberg is an assistant professor of physics and applied physiology at Georgia Tech. He earned his Ph.D. from UC, Berkeley and did his postdoctoral work at the University of Washington. Simon is a Hertz fellow and was awarded the young investigator award from the International Society of Neuroethology and a NSF biological informatics fellowship. His research is at the interface of physics and physiology, using a dynamic systems and neuromechanics approach to understand biological locomotion, motor control, and the multiscale physics of muscle.

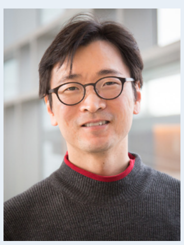
ORNL/Georgia Tech Joint Workshop in Neutron Science and Scattering

January 27, 2016

Oak Ridge National Laboratory Presenters' Biographies

Souleymane Omar Diallo, omardiallos@ornl.gov

Dr. Diallo is an instrument scientist on the ORNL BASIS instrument, SNS beam line 2. His current scientific interests are in the field of biological physics; in particular in understanding the relationship between the structure and dynamics of proteins or other complex macromolecules (polymers), the water around them, and their biological functions under varying physiological and environmental conditions. He received his PhD in condensed matter physics from the university of Delaware. Prior to joining ORNL, he was a postdoctoral research associate in the neutron and X-ray scattering group at Ames Laboratory.



Changwoo Do, doc1@ornl.gov

Dr. Do is an instrument scientist on the ORNL EQ-SANS instrument, SNS beam line 6. His primary research interests are in the structure and dynamics understanding of soft materials including polyelectrolytes, water, charged micelles, and block copolymer self-assemblies. He also uses molecular dynamics to assist interpretation of neutron scattering data and to understand molecular level structure and dynamics that are complementary to the experiment. Changwoo studied physics at KAIST in South Korea and at the Massachusetts Institute of Technology, and received a Ph.D. in nuclear and quantum engineering at KAIST.

William Heller, hellerwt@ornl.gov

Dr. Heller is a physicist and the lead instrument scientist on the ORNL EQ-SANS instrument, SNS beam line 6. His primary research interests are in the structure of biomembranes and their interactions with proteins and peptides. William also develops methods and software for modeling small-angle scattering data. Heller studied physics and mathematics at the University of Nebraska, Lincoln, and received a Ph.D. in physics from Rice University.

Mike Fitzsimmons, fitzsimmonsm@ornl.gov

Dr. Fitzsimmons is the group leader of the Thin Films and Nanostructures, Quantum Condensed Matter Division, ORNL Neutron Sciences Directorate. Fitzsimmons' scientific research involves neutron and X-ray scattering studies of interfaces in complex materials and nanocomposites. He received his Ph.D. from Cornell University. He worked at Los Alamos National Laboratory, served as an affiliate of the University of California at San Diego, and was a four-time visiting researcher at the Université H. Poincaré Vandœuvre les Nancy, France. Fitzsimmons is presently the Treasurer and an Officer of the Board of Directors for Materials Research Society. Fitzsimmons is a fellow of the American Physical Society and the Neutron Scattering Society of America.

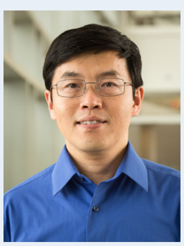
OAK RIDGE National Laboratory

Georgia Institute of Technology®

Andrey Kovalevsky, kovalevskyay@ornl.gov
Dr. Kovalevsky is a macromolecular crystallographer, biochemist and instrument scientist on the IMAGINE instrument, HFIR beam line CG-4D. His current research focuses on the atomic level understanding of enzyme function, drug binding, and drug resistance, including the effects of molecular dynamics, utilizing macromolecular X-ray and neutron crystallography and other biophysical methods. He held a Director's Postdoctoral Fellowship while at Los Alamos National Laboratory (LANL), where he was awarded the Postdoctoral Distinguished Performance Award. He also held a position as a Staff Scientist at LANL. Kovalevsky studied organic chemistry and crystallography at Kharkov State University, Kharkov, Ukraine, receiving an M.Sc. with honors, and received his Ph.D. in Physical Chemistry from the State University of New York at Buffalo. He studied macromolecular crystallography, biochemistry and molecular biology while working as a Postdoctoral Associate at Georgia State University, and then as a Postdoctoral Fellow at LANL.

Greg Smith, smithgs1@ornl.gov
Dr. Smith is the group leader for the Structure and Dynamics of Soft Matter Group, in the Biology and Soft Matter Division, ORNL Neutron Sciences Directorate. Smith's current research includes studies of the structure and interactions in biomimetic membranes and soft colloids. Smith received a Ph.D. in condensed matter physics from Iowa State University. He worked at Los Alamos National Laboratory as an instrument scientist and deputy group leader. Smith is a Fellow of the American Physical Society and the Neutron Scattering Society of America.

Alan Tennant, tennantda@ornl.gov
Dr. Tennant is the chief scientist for Oak Ridge National Laboratory's Neutron Sciences Directorate and director of the Joint Institute for Neutron Sciences, a partnership between ORNL and the University of Tennessee, Knoxville. Tennant studied physics at the University of Edinburgh, Scotland, and earned his Ph.D. at the University of Oxford. He served as a professor at the Technical University, Berlin, and institute director in the field of magnetism at the Helmholtz Center Berlin. Tennant received the Europhysics Prize for the experimental observation of magnetic monopoles in spin ice in 2012.



Xiaoping Wang, wangx@ornl.gov
Dr. Wang is an instrument scientist co-responsible for the TOPAZ single crystal diffractometer, ORNL Spallation Neutron Source beam line 12. He received his Ph.D. in inorganic chemistry from Texas A&M University in 1998, where he did his graduate work with Professor F. Albert Cotton. Wang's primary research interest is applications of neutron single crystal crystallography in chemistry and materials science. He was chair-elect and chair of the Small Molecule SIG of the American Crystallographic Association in 2006 and 2007. Dr. Wang is co-author of more than 120 research papers published in peer-reviewed journals.

The next generation of materials research

SNS site including support facilities and the Center for Nanophase Materials Sciences

Purpose: Provide intense pulsed neutron beams for research on the structure and dynamics of materials in fields such as physics, chemistry, materials science, and biology.

Sponsor: US Department of Energy, Office of Basic Energy Sciences

Features:
- Completed in 2006; user program began in 2007
- Designed to operate at 1.4 MW beam power at 60 Hz
- Provides 4,500 hours of beam time for users annually
- Two proposal calls held annually
- By 2015, 19 instruments will be available in the User Program
- Capacity for up to six additional instruments
- More than 1,500 users conduct approximately 450 experiments annually at SNS

Users: Scientists and engineers from universities, industries, and government laboratories around the world.

SNS

OAK RIDGE National Laboratory

U.S. DEPARTMENT OF ENERGY Office of Science

www.ornl.gov/science-discovery/neutron-science

07-G00050F/gim

Spallation Neutron Source

The Spallation Neutron Source (SNS) gives researchers more detailed information on the structure and dynamics of physical and biological materials than ever before possible. This accelerator-based facility provides the most intense pulsed neutron beams in the world. Scientists are able to count scattered neutrons, measure their energies and the angles at which they scatter, and map their final positions. SNS enables measurements of greater sensitivity, higher speed, higher resolution, and in more complex sample environments than have been possible at existing neutron facilities.

Future Growth

SNS was designed from the outset to accommodate a second target station, effectively doubling the capacity of the accelerator infrastructure to drive science using neutrons. This would enable the addition of 20-24 neutron scattering instruments and correspondingly expand the number of users, broadening scientific impact in nanoscience, biomaterials, energy storage, structural materials, and magnetic systems.

User Program

Each year the User Office issues two calls for proposals. Submissions are peer-reviewed by external panels, with recommendations based on scientific and technological impact and the experience of the research team. Experiments are also reviewed for feasibility and safety. Those with the highest potential for science impact are approved by the Neutron Sciences Directorate and scheduled for instrument access.

Meeting the needs of users is paramount at SNS. To find out more or to provide input on the Neutron Sciences User Program, contact neutronusers@ornl.gov or visit www.ornl.gov/science-discovery/neutron-science.

Additional Nearby Facilities

Research capabilities at SNS are enhanced by the proximity of other ORNL user facilities, most with the same access and training requirements. One of our major goals is to improve integration between the facilities, making it easier for users to access the support they need. Major user facilities at ORNL include the following:

- High Flux Isotope Reactor
- Center for Nanophase Materials Sciences
- Oak Ridge Leadership Computing Facility
- Center for Structural Molecular Biology
- Bio-Deuteration Laboratory

Located at the SNS site are two additional facilities that benefit users:

- The Joint Institute for Neutron Sciences, established in conjunction with The University of Tennessee, is an intellectual center for neutron users.
- The ORNL Guest House accommodates overnight visits for users.

HFIR site including support facilities

Multiple mission, high-performance reactor

Purpose: Provide intense continuous neutron beams for research on the structure and dynamics of materials in fields such as physics, chemistry, materials science, and biology.

Sponsor: US Department of Energy, Office of Basic Energy Sciences

Features:
- 85 MW steady-state source
- Peak thermal flux of 2.6 x 10^{15} neutrons/cm^2/sec
- Provides 3,400 hours of beam time for users annually
- Two proposal calls held annually
- Twelve neutron scattering instruments
- More than 1,000 users conduct 300 experiments annually
- Over 1,300 materials and neutron activation analysis irradiations annually
- Reliable source of unique commercial and medical isotopes

Users: Scientists and engineers from universities, industries, and government laboratories.

High Flux Isotope Reactor

The High Flux Isotope Reactor (HFIR) is the highest-flux reactor-based source of neutrons in the United States. Neutrons produced by HFIR are used for neutron scattering, materials irradiation, and isotope production. HFIR's capabilities provide access to the molecular and magnetic structures and behavior of materials, including high-temperature superconductors, polymers, metals, and biological samples. Because of the very high flux, the reactor is a unique resource used for medical, industrial, and research isotope production; research on severe neutron damage to materials; and neutron activation to examine trace elements.

HFIR underwent the most dramatic transformation in its 40-year life in recent years. The facility operates with high predictability, including the liquid hydrogen cold source and a new neutron guide hall housing cold-neutron instruments.

User Program

Each year the User Office issues two calls for proposals. Submissions are peer-reviewed by external panels, with recommendations based on scientific and technological impact and the experience of the research team. Experiments are also reviewed for feasibility and safety. Those with the highest potential for science impact are approved by the Neutron Sciences Directorate and scheduled for instrument access.

Meeting the needs of users is paramount at HFIR. To find out more or to provide input on the Neutron Sciences User Program, contact neutronusers@ornl.gov or www.ornl.gov/science-discovery/neutron-science.

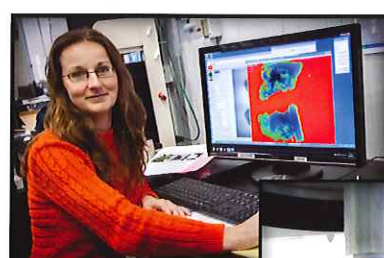
Additional Nearby Facilities

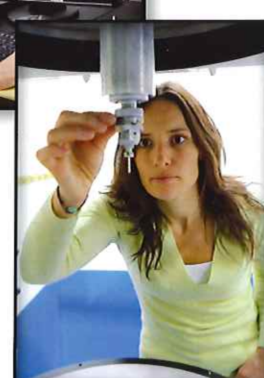
Research capabilities at HFIR are enhanced by the proximity of other ORNL user facilities, most with the same access and training requirements. One of our major goals is to improve integration between the facilities, making it easier for users to access the support they need. Major user facilities at ORNL include the following:

- Spallation Neutron Source
- Center for Nanophase Materials Sciences
- Oak Ridge Leadership Computing Facility
- Center for Structural Molecular Biology
- Bio-Deuteration Laboratory

Located at the SNS site are two additional facilities that benefit users:

- The Joint Institute for Neutron Sciences, established in conjunction with The University of Tennessee, is an intellectual center for neutron users.
- The ORNL Guest House accommodates overnight visits for users.





Neutron Sciences Call for Proposals Due April 13, 2016

Proposals for beam time at Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) will be accepted via the web-based proposal system until

11:59 a.m. (EDT) Noon, Wednesday, April 13, 2016.

This call is for experiments anticipated to run from July–December 2016.

Information and instructions

To learn more about submitting a proposal for beam time, go to neutrons.ornl.gov/users/ or directly to the proposal system at www.ornl.gov/sci/iums/ipts/. Previously submitted proposals may be used as the basis for new proposals. All proposals will be reviewed for feasibility, safety, and the potential for high-impact science. Before beginning approved experiments, users must complete access and training requirements and ensure that the appropriate user agreements are in place.

AVAILABLE INSTRUMENTS FOR GENERAL USERS

HFIR

- HB-1 Polarized Triple-Axis Spectrometer
- HB-1A Fixed-Incident-Energy Triple-Axis Spectrometer
- HB-2A Neutron Powder Diffractometer
- HB-2B Neutron Residual Stress Mapping Facility
- HB-2C US/Japan Wide-Angle Neutron Diffractometer (WAND)
- HB-3 Triple-Axis Spectrometer
- HB-3A Four-Circle Diffractometer
- CG-1D Neutron Imaging Prototype Station
- CG-2 General-Purpose SANS
- CG-3 Bio-SANS
- CG-4C Cold Neutron Triple-Axis Spectrometer
- CG-4D Image-Plate Single-Crystal Diffractometer (IMAGINE)

SNS

- BL-1A Ultra-Small-Angle Neutron Scattering Instrument (USANS)

BL-1B Nanoscale-Ordered Materials Diffractometer (NOMAD)

- BL-2 Backscattering Spectrometer (BASIS)
- BL-3 Spallation Neutrons and Pressure Diffractometer (SNAP)
- BL-4A Magnetism Reflectometer (MR)
- BL-4B Liquids Reflectometer (LR)
- BL-5 Cold Neutron Chopper Spectrometer (CNCS)
- BL-6 Extended Q-Range SANS (EQ-SANS)
- BL-7 Engineering Materials Diffractometer (VULCAN)
- BL-9 Elastic Diffuse Scattering Spectrometer (CORELLI)
- BL-11A Powder Diffractometer (POWGEN)
- BL-11B Macromolecular Neutron Diffractometer (MaNDi)
- BL-12 Single-Crystal Diffractometer (TOPAZ)
- BL-14B Hybrid Spectrometer (HYSPEC)
- BL-15 Neutron Spin Echo Spectrometer (NSE)
- BL-16B Vibrational Spectrometer (VISION)
- BL-17 Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)
- BL-18 Wide Angular-Range Chopper Spectrometer (ARCS)

For more information on any of these instruments go to neutrons.ornl.gov, or contact the Neutron Sciences User Office, neutronusers@ornl.gov or (865) 574-4600.

Oak Ridge National Laboratory is managed by UT-Battelle for the US Department of Energy.

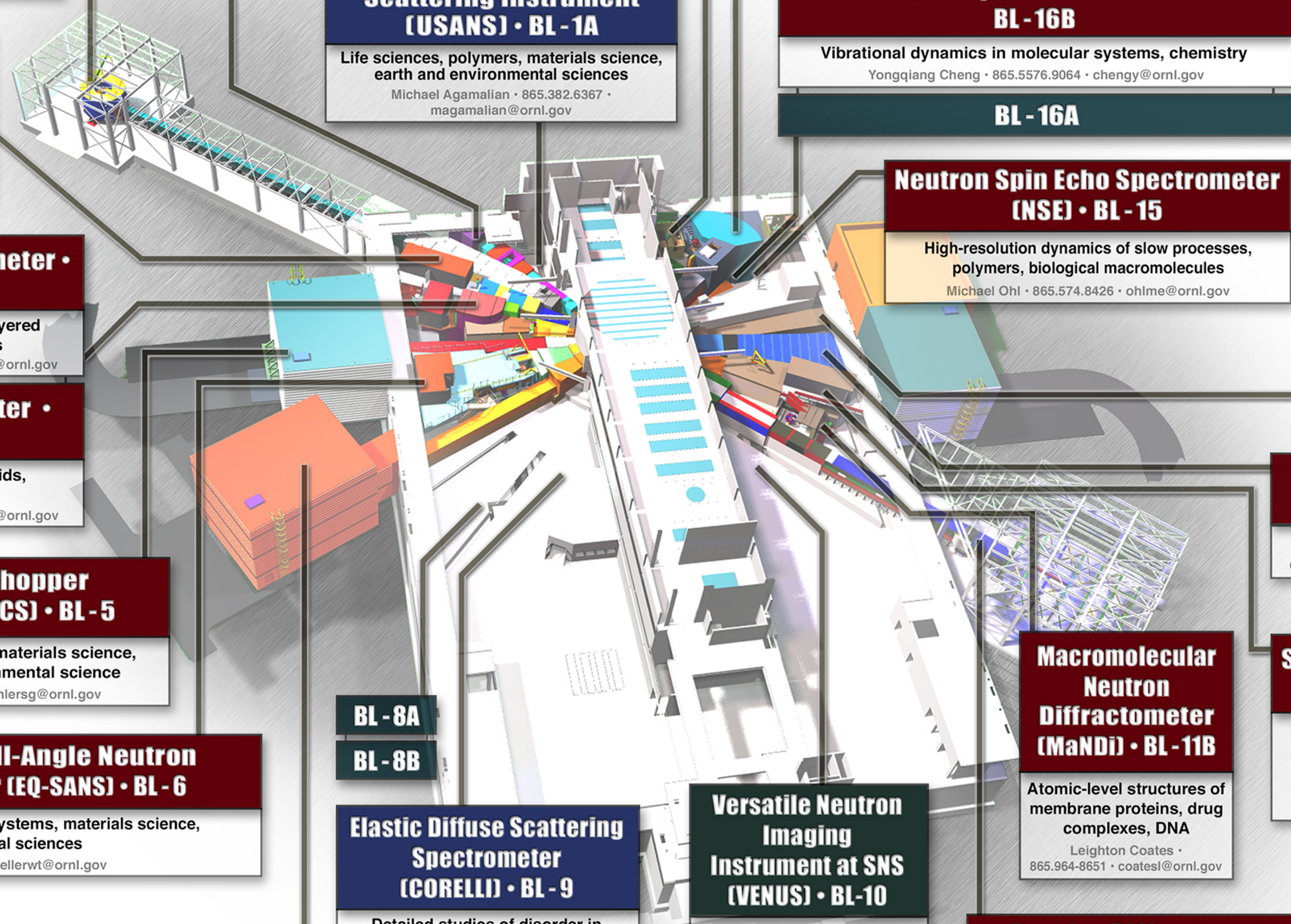
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

15-G00044B/gim

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

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

NEUTRONS.ORNL.GOV



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
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
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

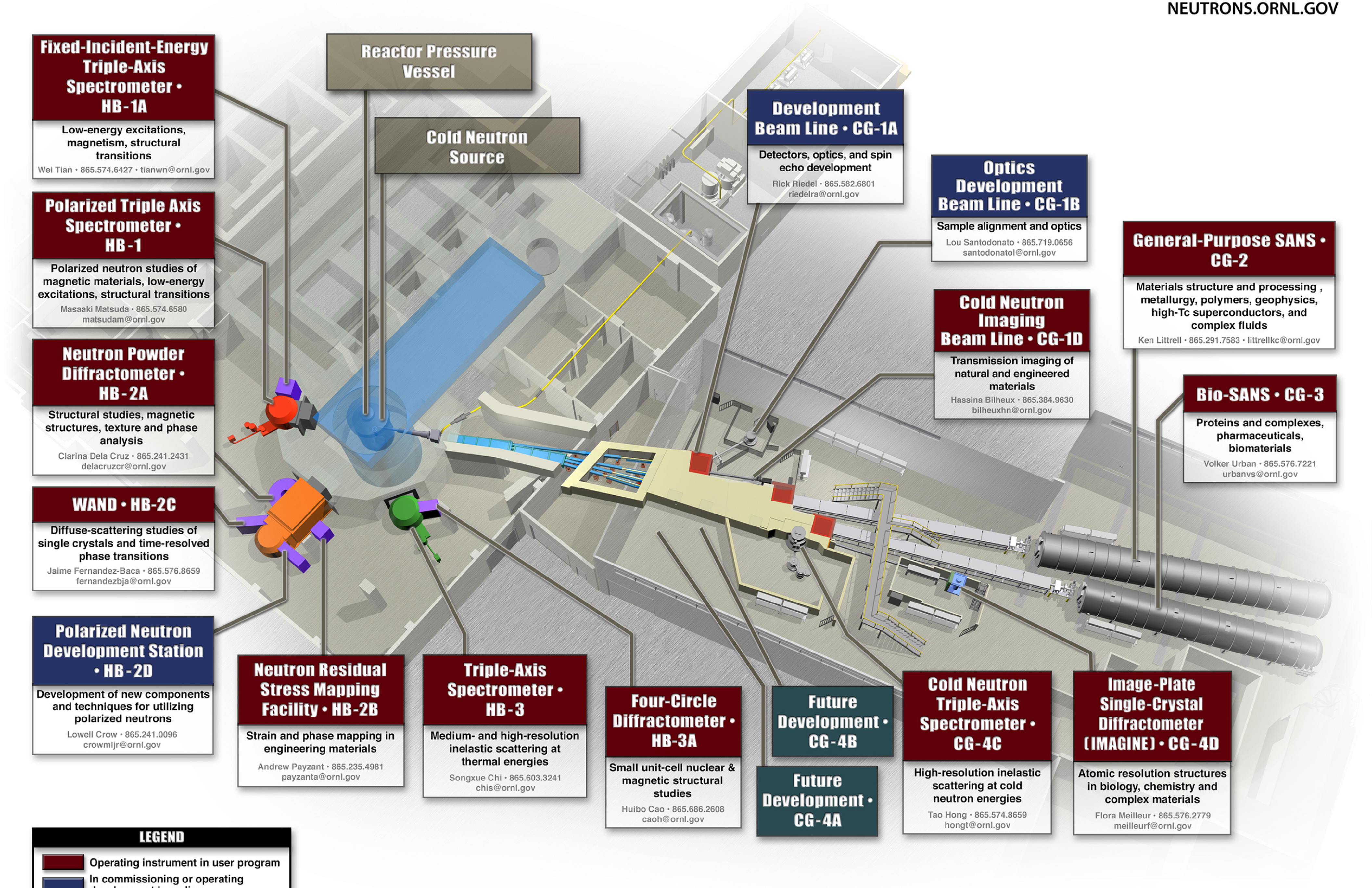
The Spallation Neutron Source is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

14-G00875A/gim

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

The United States' highest flux reactor-based neutron source

NEUTRONS.ORNL.GOV



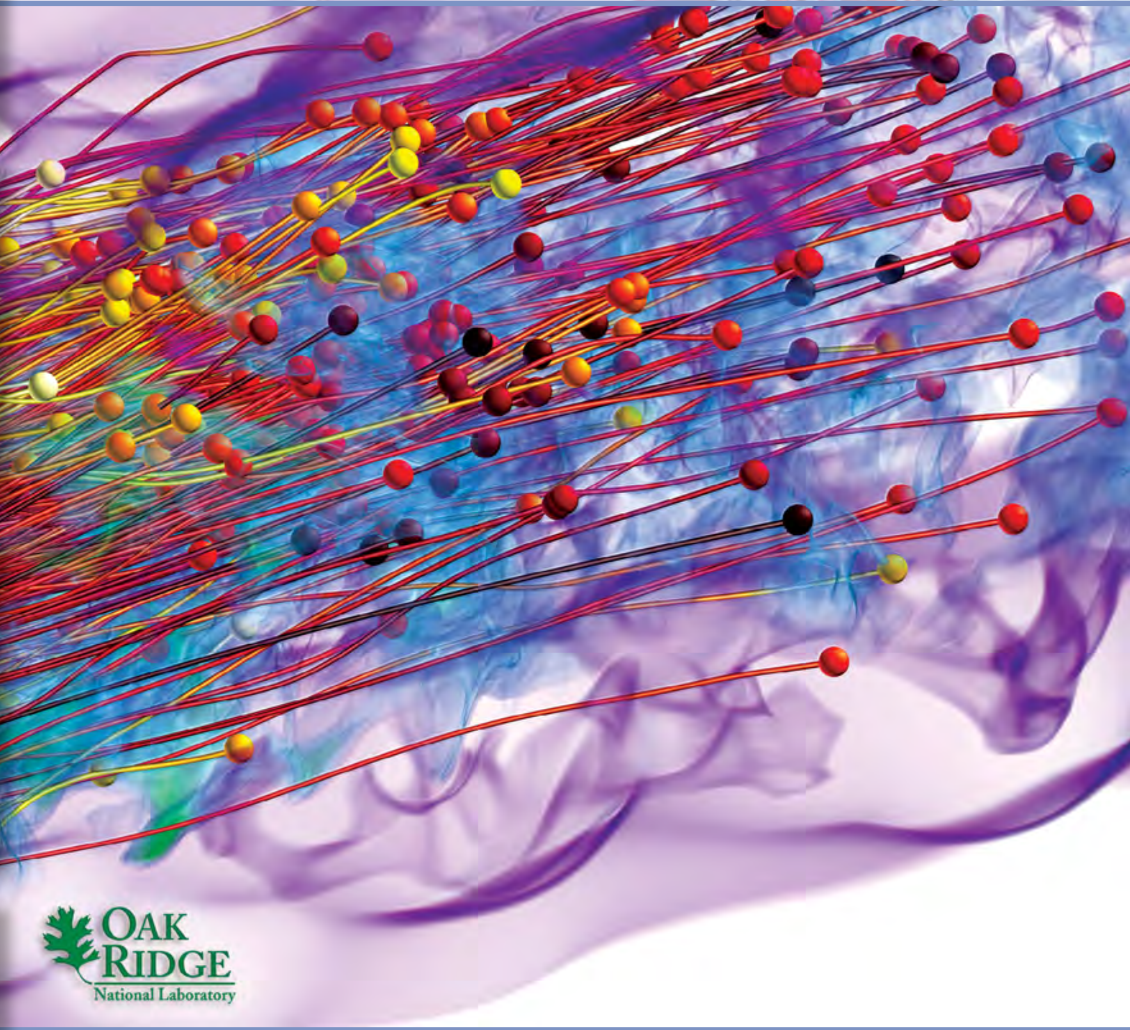
LEGEND

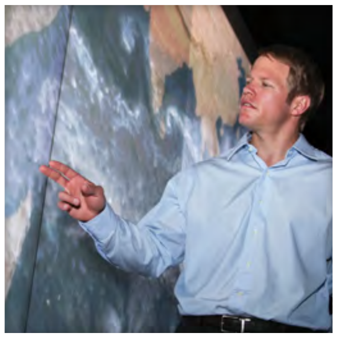
- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

14-G00872/gim

The High Flux Isotop Reactor is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

Solving Big Problems





Oak Ridge National Laboratory

Science and Technology at Oak Ridge National Laboratory

Managed by UT-Battelle for the US Department of Energy

Contents

On the cover

Background image:

In this fuel combustion simulation created on an ORNL supercomputer, colored spheres represent tracer particles that allow characterization of the turbulent mixing of ethylene and air in an engine.

Top to bottom:

Galen Shipman discusses climate simulations at a visualization wall.
Daniela Anjos prepares a sample for spectroscopic investigation.
Allison Hugh displays research findings at a visualization wall.
Sheng Dai tests electrolytes for advanced battery research.

Project Manager—Lynn Kszos

Writers—Deborah Counce, Kathy Graham, Gregory Scott Jones, Dawn Levy, Bonnie Nestor, Ron Walli, Leo Williams

Designer—Brett Hopwood

Photographers—Hassina Bilheux, Curtis Boles, Charles Brooks, Larry Hamill, Genevieve Martin, Jay Nave, Jason Richards

Stock images—iStockphoto™

Editors—Priscilla Henson, David Keim

Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the US Department of Energy under contract DE-AC05-00OR22725.

www.ornl.gov

Scientific advancement through multidisciplinary collaboration

As the largest multiprogram science and energy laboratory of the US Department of Energy, Oak Ridge National Laboratory is engaged in a wide range of activities that support DOE's mission: ensuring America's security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions. To execute these activities, ORNL integrates and applies a remarkable set of core capabilities that comprises talented staff and distinctive scientific facilities and equipment.

On the pages that follow, you will see how ORNL is focusing these resources on the delivery of scientific discoveries and technical breakthroughs that will accelerate the development and deployment of solutions in clean energy and global security, and in doing so create economic opportunity for the nation. The programs outlined here reflect an orientation to both scientific disciplines and national missions—a unique combination that characterizes ORNL and enables us to deliver national-scale solutions to problems of critical importance.

The strong partnership between DOE and UT-Battelle, LLC, which manages ORNL for the department, has created a national resource that draws outstanding researchers in a wide range of disciplines to world-class facilities where they attack fundamental scientific challenges, couple discoveries with applied research, and work with industry to translate results into commercial applications. The work of the laboratory is being performed safely and efficiently in a modern campus setting. Throughout the region ORNL is justifiably regarded as a high-value asset for innovation, education, and economic development.

Our challenge now is to sustain our leadership and build on our success. Thank you for your interest in how ORNL is helping to address some of the grand challenges facing our nation and the world.

Johnny Moore
Manager,
DOE Oak Ridge National Laboratory
Site Office

Thom Mason
Director,
Oak Ridge National Laboratory and
President and CEO, UT-Battelle, LLC

Delivering forefront science and technical breakthroughs

A history of mission-driven R&D

Oak Ridge National Laboratory was established in 1943 to carry out a critical assignment for the Manhattan Project: demonstrating the production and separation of plutonium to fuel an atomic weapon. An experimental nuclear reactor and pilot-scale chemical processing plant were constructed in the hills of East Tennessee and staffed by scientists, engineers, and technicians who worked in secrecy to complete this urgent task.

Once its wartime mission was successfully accomplished, ORNL took on a new assignment: the development of nuclear energy for peaceful purposes. The facilities and expertise assembled for the Manhattan Project expanded to support a nuclear research and development portfolio that extended from basic science to applied technology.

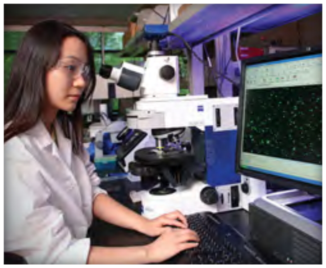
As national needs evolved, ORNL developed and applied new capabilities for understanding and solving a wide variety of energy-related problems. Today the lab conducts a broad range of R&D, primarily for the US Department of Energy, but also for other federal agencies and both public and private sponsors.

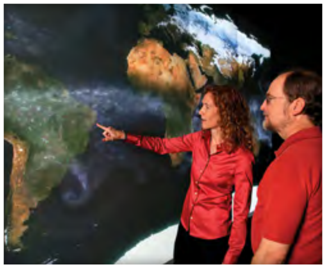
National resources for "Big Science"

DOE's 17 national laboratories occupy a unique niche in the nation's R&D enterprise, providing the resources needed to perform what former ORNL director Alvin Weinberg famously called "Big Science"—large-scale, long-term R&D efforts that are outside the scope of industry or universities.

National labs are distinguished by their ability to assemble large teams of experts from a variety of scientific and technical disciplines to tackle compelling national problems. They also design, build, and operate powerful scientific facilities that are available to the international research community. They work in partnership with universities and industry to train the future science and engineering workforce and transfer the results of their R&D to the marketplace.

DOE national labs have consistently responded to national priorities with scientific and technological achievements that have improved the nation's security, quality of life, and economic competitiveness.





A focus on delivering solutions to complex challenges

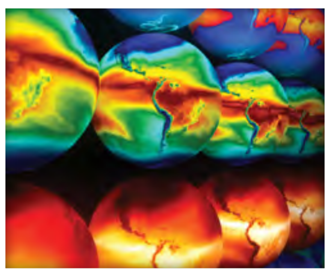
Science and technology can help us overcome many of the complex and interlocking challenges that we face as a nation in the 21st century. These challenges include ensuring our national security in a changing world, increasing the availability of clean and affordable energy, adapting to and mitigating the impacts of climate change, improving human health, and enhancing US competitiveness by encouraging innovation.

DOE has a central role in addressing these challenges. To accomplish its mission of ensuring America's security and prosperity, it relies on its national laboratories, including ORNL, for transformative science and technology solutions to energy, environmental, and nuclear challenges.

ORNL is DOE's largest multiprogram science and energy laboratory, with scientific and technical capabilities spanning the continuum from basic to applied research. These resources enable the lab to tackle an exceptionally wide range of R&D assignments, from fundamental nuclear physics to applied R&D on advanced energy systems. In addition, ORNL has a well-deserved reputation for combining insights from fundamental science with an in-depth technical understanding of applied systems to deliver practical solutions to real-world problems.

ORNL aggressively pursues opportunities to put these solutions to work, often collaborating with industry to accelerate their deployment by the private sector. Products as diverse as radiation detectors, thin-film batteries, high-efficiency heat pumps, and high-performance steel alloys have emerged from the lab's R&D.

Transfer of these and other innovations to the private sector has created new industries in the United States, resulted in substantial cost savings for companies and consumers, and provided good jobs for Americans. As global competition ramps up, ORNL will continue to attack the fundamental research challenges posed by DOE's missions and to carry out the translational research required to accelerate the delivery of solutions to the marketplace.



Developing energy solutions for a sustainable future

It heats and cools our homes, charges our smartphones, fuels our vehicles, and powers our factories. Energy is an essential part of our lives, and the need for more is escalating along with populations, economic development, and standards of living around the globe. Yet challenges exist.

Today fossil fuels supply more than 80 percent of the world's energy. Rising demand is leading to higher prices for these finite resources and ultimately consumer goods. It is also increasingly clear that the carbon emissions released by burning fossil fuels take an unacceptable toll on the environment.

To solve these pressing global challenges, ORNL carries out focused R&D to understand and reduce the impacts of our energy choices and to find more cost-effective and environmentally friendly ways to produce and use energy. The lab's clean energy R&D brings together experts in biological and environmental sciences, advanced materials, neutron sciences, nuclear science and engineering, and high-performance computing.

For example, ORNL researchers are developing new materials, advanced control systems, and innovative processes and techniques to improve the efficiency of energy technologies. Laboratory advances in lightweighting materials, such as high-strength steel alloys and low-cost carbon fiber, are helping automakers meet higher vehicle fuel-efficiency standards. ORNL also works with industry to develop high-efficiency home appliances and combine them with advanced building materials and construction techniques to build houses that produce as much energy as they consume. A new Manufacturing Demonstration Facility is assisting US industry in developing cutting-edge solutions that use less energy, reduce waste, and strengthen the nation's manufacturing base.

Accelerating biofuels

The BioEnergy Science Center (BESC), established by DOE in 2007, plays a key role in ORNL clean energy research by accelerating progress toward a viable biofuels market. BESC's goal is to enable revolutionary breakthroughs that allow the use of lignocellulosic biomass—mainly wood and grass—to produce transportation fuels.

Plant geneticist Wellington Muchero examines phenotypic traits of *Populus* transgenic lines grown in a greenhouse at ORNL.

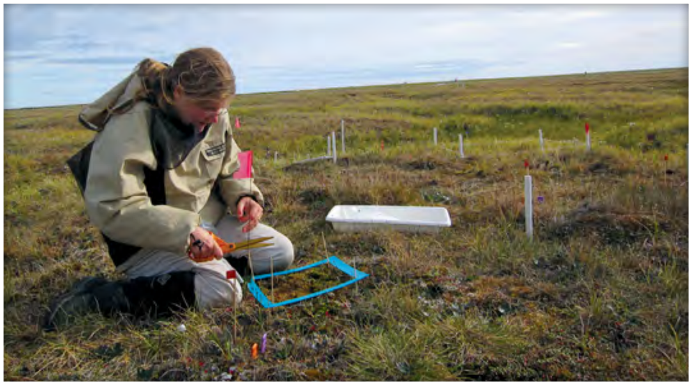
Transportation unplugged

ORNL is dropping the cord in electric vehicle charging in favor of wireless power transfer that is safer and more convenient. Whether stationary or on the go, the technology's magnetized coil system wirelessly transfers electricity to a vehicle's onboard battery pack while it's positioned over an embedded charging sensor.

Researcher Steven Campbell demonstrates an electric vehicle being wirelessly charged using ORNL technology.

The lab's R&D on low-carbon energy technologies spans nuclear fission, nuclear fusion, and renewable sources including solar, wind, hydropower, geothermal, and biomass. Our scientists and engineers conduct research to support the US nuclear power industry, which supplies about 20 percent of the nation's electricity; develop advanced concepts that will enhance the safety and reliability of the next generation of nuclear power plants; and work with international partners to harness the power of the stars by generating fusion energy on earth.

ORNL researchers are also working to expand the nation's renewable energy options. Expertise in biology, chemistry, physical and computational sciences, and engineering is applied to developing new bioenergy crops and transforming them into biofuels and bio-based products that can reduce our nation's dependence on imported petroleum. Fundamental studies of batteries are coupled with R&D on manufacturing and processing to produce durable and affordable energy storage systems that can provide US industry with a competitive advantage in the global marketplace.



ORNL researcher Victoria Sloan participates in a vegetation harvest and active-layer soil sampling exercise in Barrow, Alaska. Data will be used to improve the predictive capacity of Earth system models.

ORNL has explored the impacts of energy production, distribution, and use for decades, but this work has taken on new importance with growing evidence of climate change linked to fossil fuel consumption. Multidisciplinary research at the lab's Climate Change Science Institute is strengthening our understanding of climate change through observation and experiment, developing high-resolution climate models, and providing input to policy decisions that address societal and ecological consequences.

ORNL Capabilities Vital to Clean Energy

Advanced computer science • Applied materials science and engineering • Applied nuclear science and technology • Biological systems science • Chemical and molecular science • Chemical engineering • Climate change science • Computational science • Condensed matter physics and materials science • Large-scale user facilities/advanced instrumentation • Plasma and fusion energy sciences • Systems engineering and integration • Visualization and data

Safeguarding the nation through science and technology

As threats to our national and global security become more complex, varied, and unpredictable, ORNL's scientific and technical resources are being applied to deliver solutions to the most pressing security challenges, from weapons of mass destruction to cyber warfare. The remarkable diversity of these resources provides the lab with the tools needed to solve difficult problems in nuclear nonproliferation, homeland security, national defense, and intelligence.

Work to restrict the proliferation of nuclear weapons and weapons-grade materials builds on ORNL's seven decades of experience with nuclear science and technology. Lab researchers also develop tools and techniques for finding illicit nuclear devices such as "dirty bombs," locating stolen nuclear weapons, and verifying international agreements to dismantle nuclear warheads.

Researchers at ORNL work with federal, state, and local agencies to develop and deploy technologies to improve the ability to detect, prevent, respond to, and recover from acts of terrorism as well as natural disasters. In addition to nuclear detection technologies, the lab is providing new ways to identify small quantities of explosives, hazardous chemicals, and biological materials. ORNL also develops systems for threat assessment, risk awareness, and emergency planning and response, as well as new capabilities for first responders.

The lab meets the needs of the military by addressing specific scientific and technical challenges facing the US Department of Defense, in terms of both current and future war-fighting needs and efforts to transform military services. These challenges call for the application of capabilities across ORNL's research directorates. The lab's contributions to military programs span logistics and transportation management,

Simulation and cybersecurity

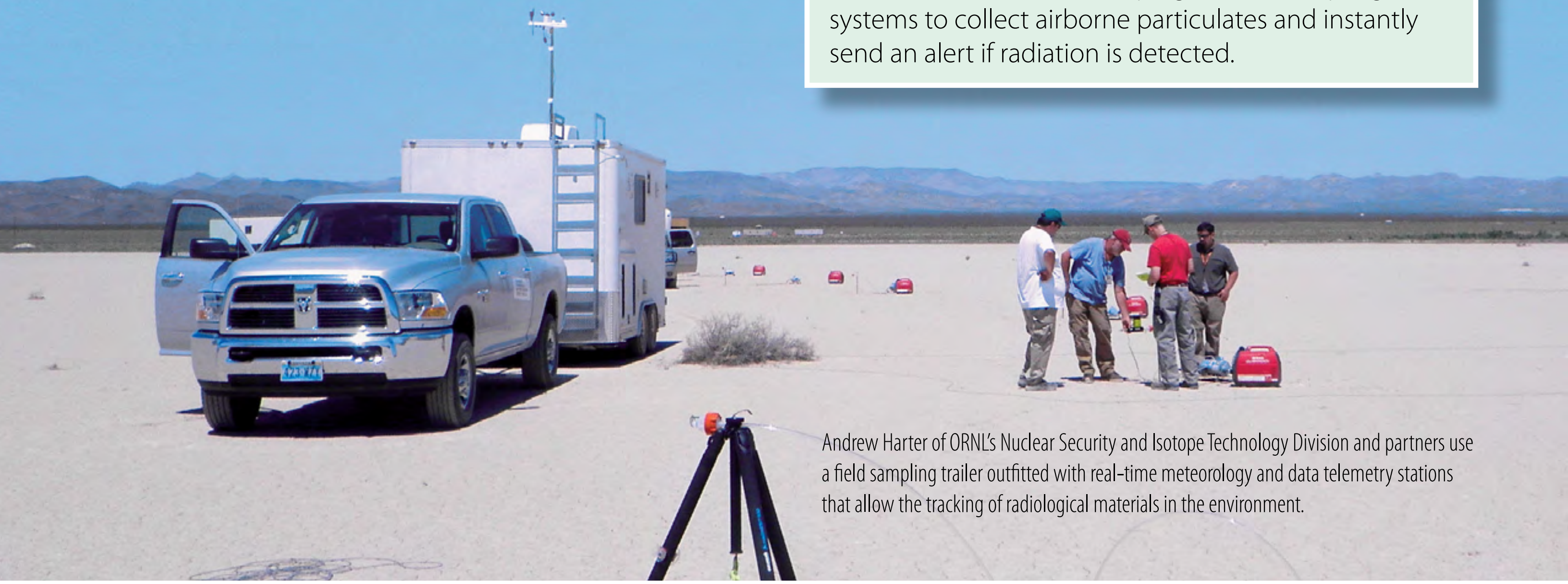
Sophisticated modeling and simulation tools are helping ORNL pinpoint potential vulnerabilities and stay ahead of attempts to launch a cyber attack. By combining simulated attacks on real-world network components with large-scale modeling and simulation, researchers can evaluate cybersecurity threats quickly and cost-effectively. Failing to meet the cybersecurity threat head-on could have dire consequences for the nation's military, banking institutions, businesses, energy producers and distributors, and others who depend on integrated computer networks.

defense against chemical and biological weapons, sensor miniaturization and communication, robotics, and special materials such as carbon fiber and titanium.

ORNL's exceptional resources for computing and computational sciences are increasingly being used to meet the needs of the military and the US Department of Homeland Security. The lab's capabilities and expertise in advanced design, simulation, and modeling are applied to challenges from the design of advanced aircraft to the analysis of large volumes of data. An area of particular interest is cybersecurity: providing the tools needed to protect critical digital infrastructure against persistent and sophisticated threats with the potential to shut down the power grid or disrupt the economy.

Nuclear forensics

Tools, techniques, and expertise in nuclear fuel cycle research gained over seven decades are helping ORNL scientists control and track nuclear bomb-grade materials to be sure they don't fall into the wrong hands. Among the leading-edge technologies used by researchers are high-resolution techniques that allow analysis of radiation detector data in stunning detail. Researchers are also developing aerosol sampling systems to collect airborne particulates and instantly send an alert if radiation is detected.

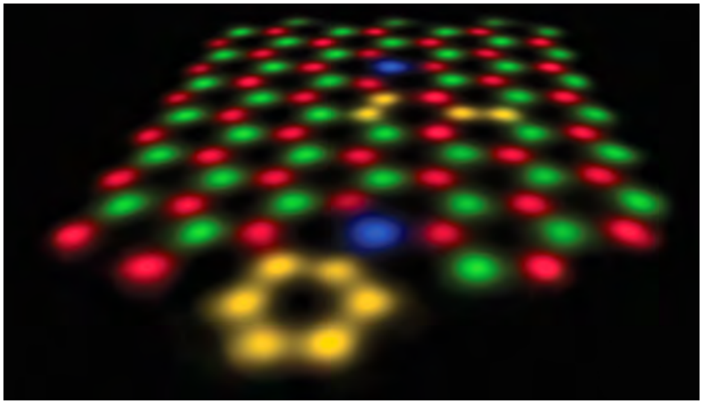


Andrew Harter of ORNL's Nuclear Security and Isotope Technology Division and partners use a field sampling trailer outfitted with real-time meteorology and data telemetry stations that allow the tracking of radiological materials in the environment.

Creating the stuff from which tomorrow will be made

To create advanced energy systems, it's essential that scientists discover and exploit the unique properties of materials. ORNL has one of the nation's most comprehensive materials research programs, which positions the lab to contribute to American initiatives in clean energy, national security, and industry.

For instance, lightweight materials are fundamental to the future of transportation and other energy-related fields. By creating new polymer composites with novel properties, ORNL is ushering in a new era of lighter vehicles that consume less fuel yet are far safer than today's cars, trucks, airplanes, and ships. And by exploiting materials that exhibit unique magnetic and electric properties, ORNL is helping the country move toward a new age of electronics in which devices such as cellular phones and tablets could exceed current data storage by a factor of thousands, making all the data on an iPhone fit in a device the size of your pupil. Other lab initiatives include understanding and manipulating materials at the nanoscale—about the size of a water molecule—and developing materials that could increase the efficiency and reliability of systems for power generation, storage, distribution, and use, such as batteries.



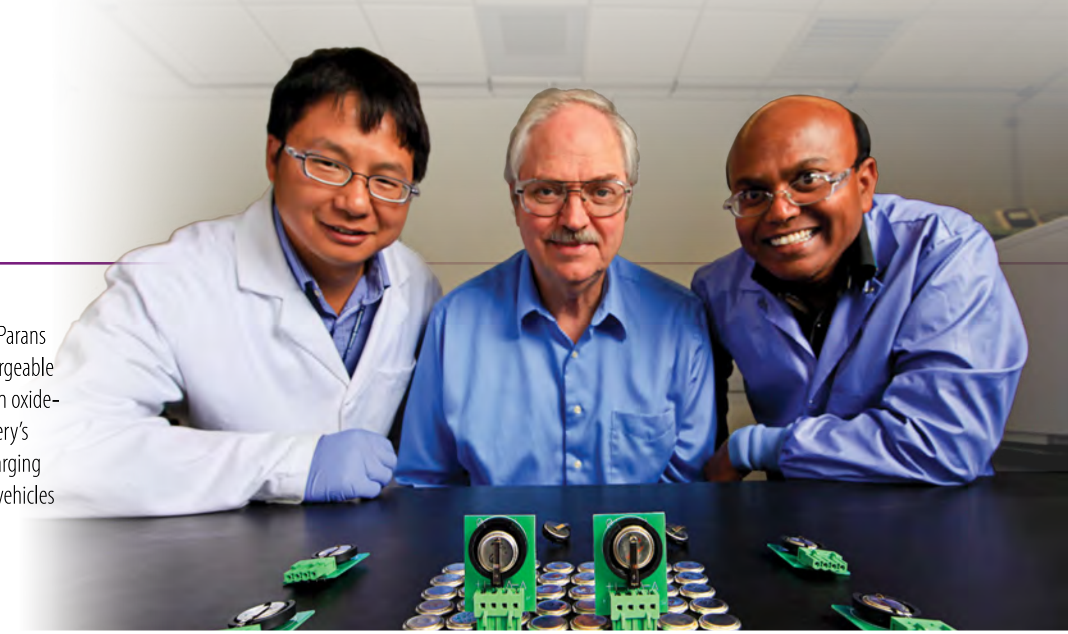
ORNL's expertise in microscopy allows researchers to visualize individual atoms 100,000 times smaller than a human hair. In this color-enhanced image, atoms of boron (red) and nitrogen (green) are shown in a single layer of boron nitride, along with the contaminants carbon (yellow) and oxygen (blue), a level of detail that allows scientists to tailor new materials for electronics and other energy applications. This image was made using ORNL improvements to aberration-corrected scanning transmission electron microscopy.

The future of manufacturing

DOE's first Manufacturing Demonstration Facility was established at ORNL to help industry adopt new technologies that reduce life-cycle energy use and greenhouse gas emissions, lower production costs, and create new products. The lab's expertise helps manufacturers reduce risks and validate their investments in innovations that will create the products—and high-paying jobs—of the future in lightweight metals, stronger materials, three-dimensional printing, and more.

ORNL's materials leadership is supported by user facilities including the Center for Nanophase Materials Sciences, Shared Research Equipment Collaborative Research Center, Spallation Neutron Source, and Oak Ridge Leadership Computing Facility.

Together ORNL's resources compose the nation's most comprehensive center for materials research and interfacial chemistry (processes that occur at boundaries between, for instance, gas and liquid or gas and solid). By coupling basic and applied research, ORNL will lead the way to unprecedented performance in energy systems based on understanding and controlling structure and function at the atomic and molecular levels.

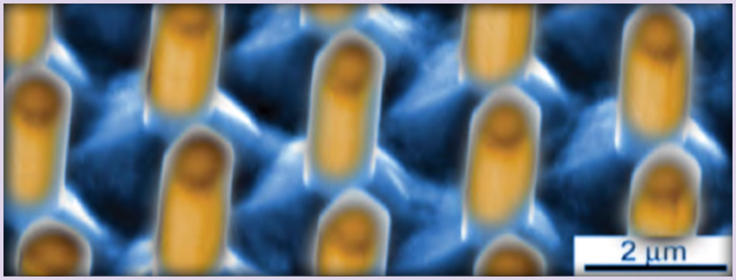


ORNL researchers Hansan Liu, Gilbert Brown, and Parans Paranthaman display an array of lithium ion rechargeable CR2032 coin cells made with mesoporous titanium oxide-based anodes. These materials can increase a battery's power and safety, while dramatically reducing charging time, making them well suited for hybrid electric vehicles and other high-power applications.

Achieving ultimate strength

Through a process known as directional solidification, ORNL researchers have grown materials in nearly perfect "pillars" a fraction of the width of a human hair. When tested, these materials had strength near their achievable limits, which is far higher than the roughly 10 percent of achievable strength found in similar materials made by traditional methods. This discovery points to a new direction for high-performance materials designed to function in extreme high-temperature and high-stress environments. By doing so it offers the possibility of significantly increasing the operating temperature—and therefore the efficiency—of such products as turbines and tremendously decreasing the amount of material required to construct strong buildings, bridges, and automobiles.

Easo George and Hongbin Bei with the ORNL high-temperature optical floating zone furnace used to produce monocrystalline molybdenum alloy micropillars.



A false-color image of molybdenum pillars sticking out of a silicon carbide matrix. Each pillar is a nearly perfect single crystal about 1/40th the width of a human hair.

ORNL Capabilities Vital to Advanced Materials

Advanced computer science, visualization, and data • Applied materials science and engineering • Chemical and molecular science • Chemical engineering
Computational science • Condensed matter physics and materials science • Large-scale user facilities/advanced instrumentation

Accelerating research and innovation

Modeling and simulation along with data exploration have joined experiment and theory as the third and fourth pillars of science, allowing researchers who make the most of supercomputers to quickly draw conclusions from complex and copious data. ORNL's world-class computing experts are committed to offering researchers the most productive supercomputing ecosystems on the planet so they can produce ground-breaking research in data-intensive science and engineering fields such as healthcare, medicine, economics, disaster recovery, and national security. For more than a decade ORNL has managed diverse data from experiments, simulation output, human activities, sensors, and more.

Large-scale computing underpins scientific disciplines including materials science, chemistry, plasma physics, astrophysics, biology, climate research, nuclear fission, and applied mathematics. ORNL deploys and operates leadership-class supercomputers including the DOE Office of Science's Titan, the National Science Foundation's Kraken, and the National Oceanic and Atmospheric Administration's Gaea. Industrial, academic, and government researchers worldwide use ORNL supercomputers and support systems for data generation, analysis, visualization, and storage to illuminate phenomena that are often impossible to study in a laboratory, such as climate impacts of energy use, fusion in a reactor not yet built, and galaxy formation.

Simulations allow virtual testing of prototypes before their actual construction, enabling compression of product design cycles and lower costs for vehicle engines, airplane wings, and power plants. In fields from disaster relief to the electric grid, simulations provide insight to inform action. They speed solutions that help improve electrochemical energy storage

Fuel efficiency

SmartTruck Systems engineers used the Oak Ridge Leadership Computing Facility (OLCF) and a National Aeronautics and Space Administration (NASA) application code to study airflow around long-haul trucks and to design trailer add-ons that dramatically decreased drag, saving an estimated $5,000 annually in fuel costs per vehicle.

Supercomputer simulations guided the design of BMI's SmartTruck UnderTray components, which improve fuel mileage by 7 to 12 percent. *Image courtesy of BMI Corp.*

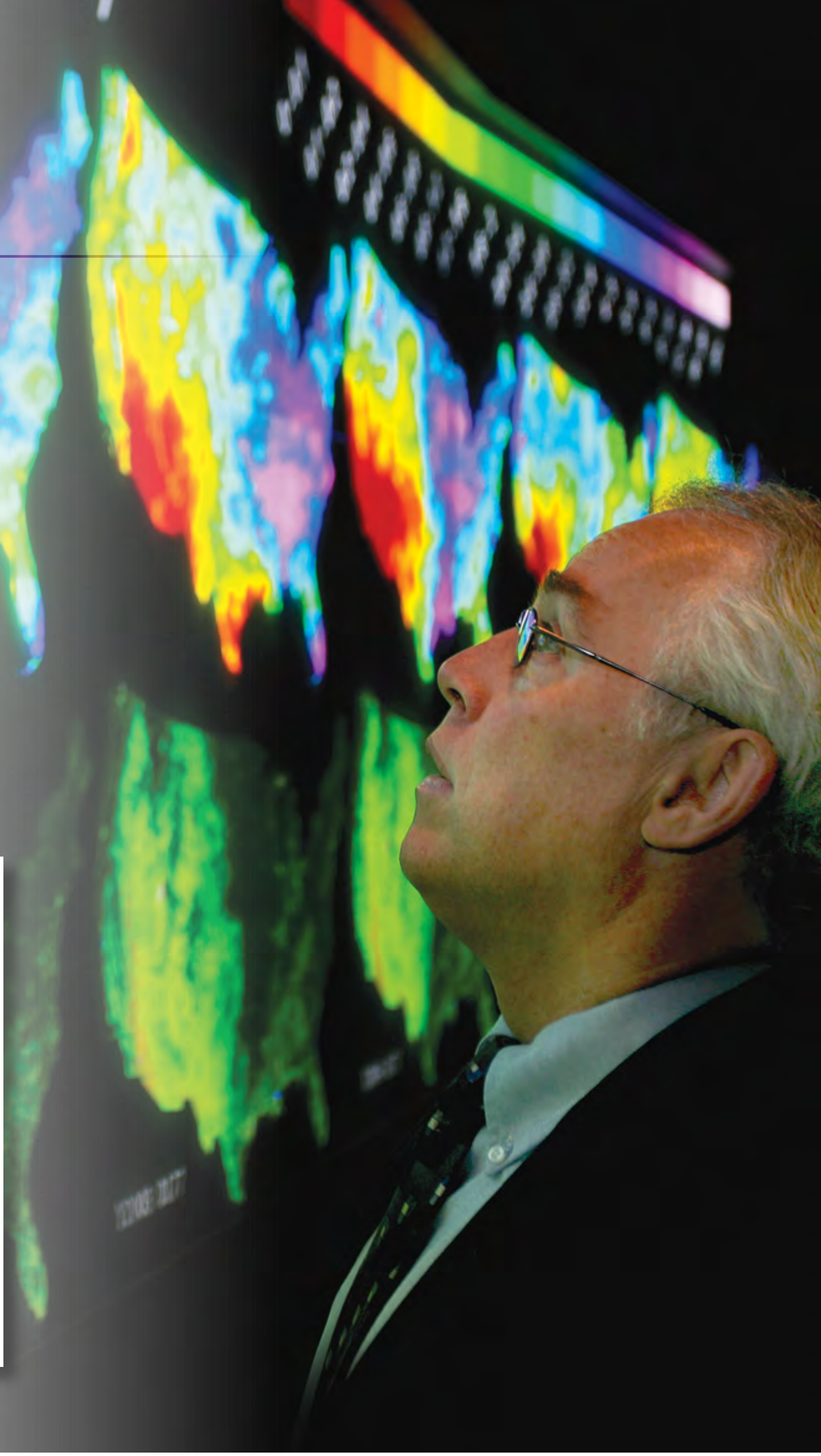
in batteries, the ability of solar cells to produce electricity, the efficiency of the nuclear fuel cycle, and the commercial viability of cellulosic biofuels.

Simulations helped create an innovative supercapacitor, forced rewriting of textbooks by revealing how pulsars get their spins, and elucidated the molecular mechanism of Parkinson's disease.

Using supercomputing resources at ORNL, researchers have helped the Federal Bureau of Investigation and the US Department of Defense assess terrorist threats. ORNL is also collaborating with the Centers for Medicare & Medicaid Services (CMS) to prototype a Knowledge Discovery Infrastructure that would give a broad range of stakeholders easier and more complete access to a CMS data center.

World-leading computing

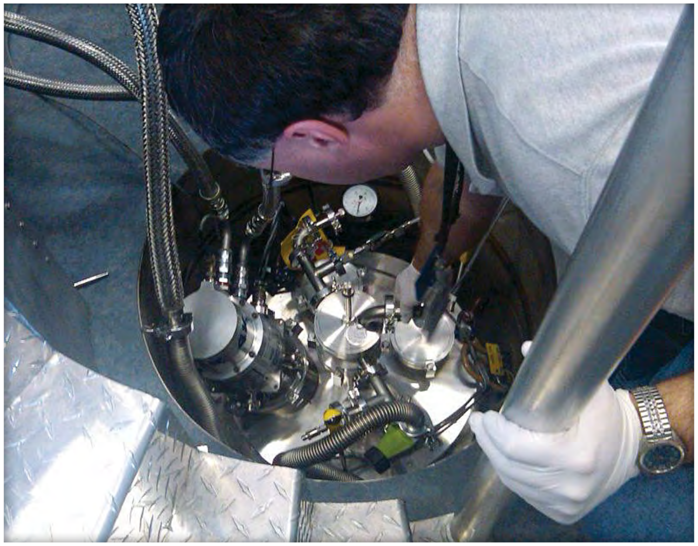
Titan—#1 for speed and #3 for energy efficiency on global rankings of supercomputers—combines traditional central processing units with high-performance graphics processing units. With a peak performance of 27 petaflops, it increases realism in simulations and enables virtual experiments, such as global-scale seismology, that were previously impossible due to the vast scale and time demands of the simulations.



James Hack, director of the National Center for Computational Sciences and head of the Climate Change Science Institute at ORNL, views climate simulations. Leadership-class supercomputers run simulations of changes in atmosphere, oceans, land, and ice that help build knowledge of the Earth system.

Revealing the mysteries of materials

Scientific investigation with neutrons gives researchers unprecedented capabilities for understanding the structure and properties of materials important in biology, chemistry, physics, and engineering. ORNL provides two of the most powerful neutron science facilities in the world—the Spallation Neutron Source and the High Flux Isotope Reactor. SNS produces the world's most intense pulsed neutron beams, and HFIR produces one of the brightest steady-state neutron streams on Earth. Through materials research, scientists are discovering remarkable ways to address our energy needs, such as superconducting power cables that eliminate power-transmission losses and prevent outages, liquid transportation fuels produced from biomass, and magnetic refrigerators that use half the energy of conventional appliances.



Eugene Mamontov loads samples for the BASIS spectrometer to explore the behavior of ionic liquids—liquid salts with enormous potential for a wide range of uses in areas such as energy storage, pharmaceuticals, biofuels, and industrial processes.

To bring such technologies into common use, researchers need to be able to view materials from the atom-to-atom scale to a full systems view. Developing these advanced

Electrical production

ORNL scientists are using neutrons to figure out how to improve the ability of certain materials to generate electricity from heat produced by industrial motors or automobile exhaust and use it to power small electrical devices. It's research that can't be done without the subatomic view of materials made possible by ORNL's large research facilities.

ORNL's Spallation Neutron Source, Center for Nanophase Materials Sciences, and Joint Institute for Neutron Sciences materials requires manipulating the properties of alloys at the atomic level, and neutron scattering is a key tool in this quest.

Neutrons show where atoms are and what they are doing at scales smaller than the best electron microscopes. They let researchers see in real time how the atomic lineup in a material shifts with changes in temperature, pressure, and magnetic or electronic fields. They trace the electron motions that give materials properties such as magnetism or the ability to conduct electricity—all essential information in the quest for energy savings.

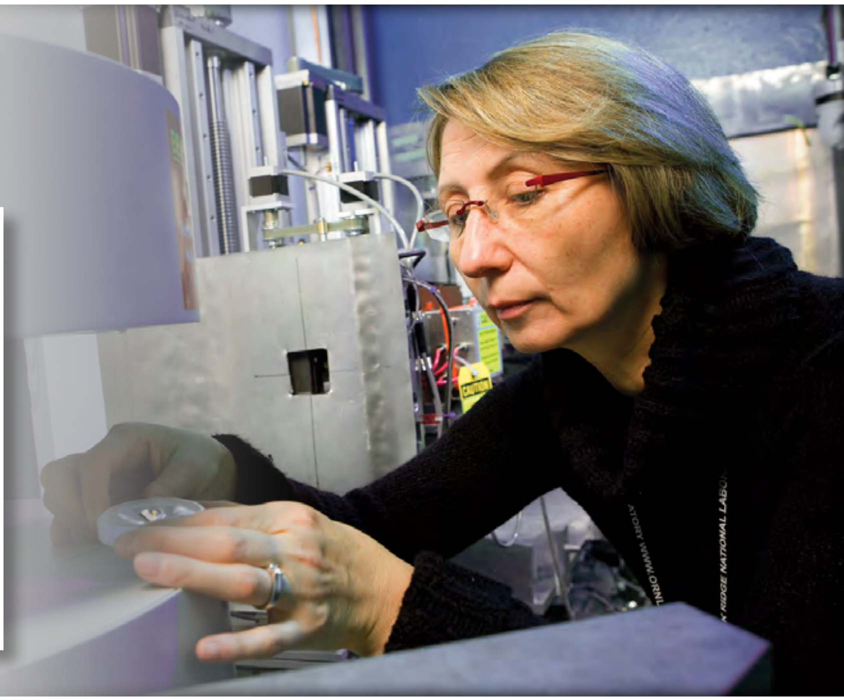
Satisfying the world's growing hunger for energy requires finding ways to use power more frugally and developing methods for sustainably producing additional energy. Neutron scattering aids the creation of new materials engineered for both purposes.

Negative thermal expansion

Materials with negative thermal expansion (NTE) contract when they're heated instead of expanding as most materials do, making them potentially useful in applications such as nanoelectronics, telescope mirrors, and dental fillings. Scientists bombarded a sample of scandium fluoride, a known NTE material, with neutrons at ORNL to discover how vibrations in its crystal structure cause NTE behavior. The understanding gained will help scientists design materials with desirable responses to temperature.

Understanding and fighting disease

The *Sindbis* virus is the prototype for insect-borne viruses that cause devastating diseases worldwide. Neutron scattering revealed how exposure to acidic conditions causes structural changes in the *Sindbis* core that help the virus attach itself to and transfer infectious RNA into human cells. The research also detailed subtle structural differences between virus particles from insect and mammalian hosts. The findings add to the understanding of how viruses infect human cells, a key to controlling the spread of insect-borne diseases.



Valeria Lauter of ORNL's Neutron Sciences Directorate mounts a sample in an electromagnet for an experiment using polarized neutrons at the Liquids Reflectometer at ORNL's Spallation Neutron Source. The reflectometer is dedicated to studies of magnetic nanostructures.

Powering the future and ensuring safety and health

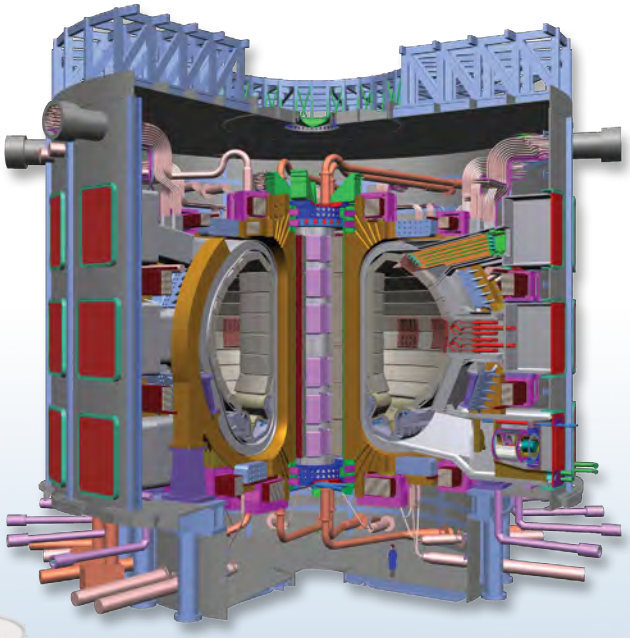
Oak Ridge helped usher in the Nuclear Age, and ORNL's scientists are leaders in using nuclear technologies and systems to improve human health; explore safer, more environmentally friendly power; and better understand the very makeup of matter.

The lab is a world leader in the production of isotopes for medical purposes and research. In fact, its isotopes have contributed to the discovery of seven new elements.

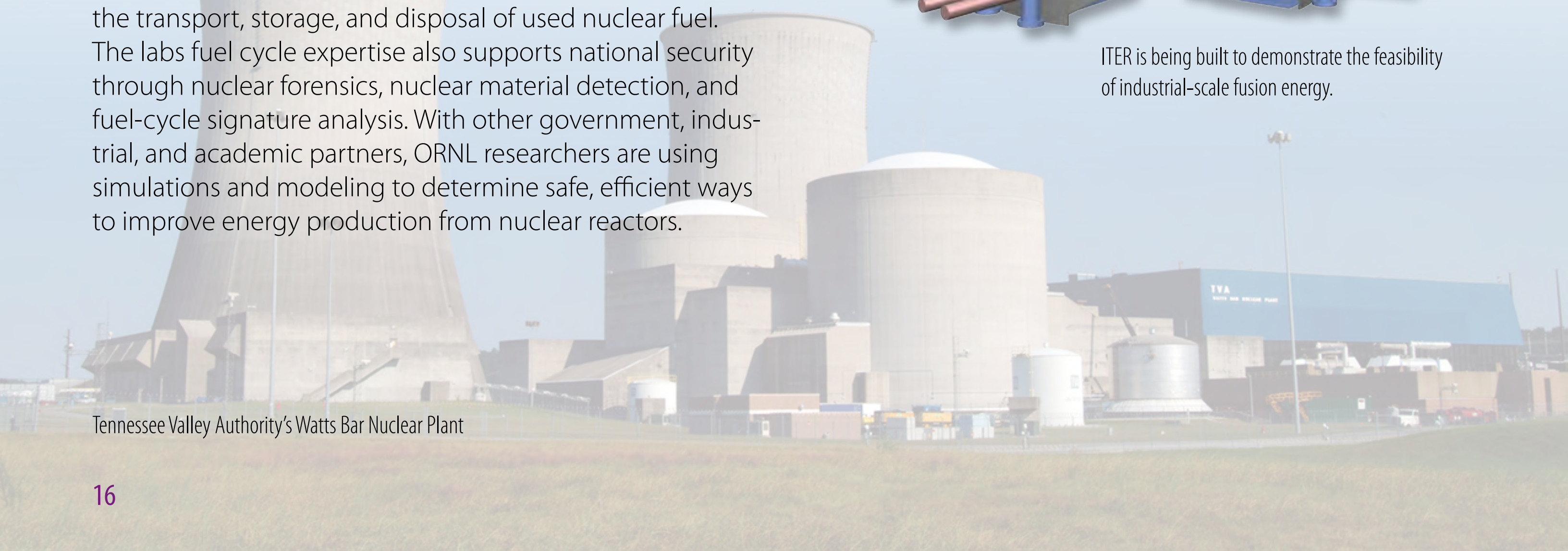
ORNL is managing US contributions to the international effort to generate fusion power at ITER, an experimental facility being built in Cadarache, France. The project will prove the scientific feasibility of fusion energy, a long-sought technology that emits no greenhouse gases, presents no risk of meltdown, produces no long-lived high-level radioactive waste, and offers no potential for nuclear proliferation.

The laboratory provides leadership in the full spectrum of research, development, and deployment of reactor and nuclear fuel cycle technologies, from fuel development to the transport, storage, and disposal of used nuclear fuel. The labs fuel cycle expertise also supports national security through nuclear forensics, nuclear material detection, and fuel-cycle signature analysis. With other government, industrial, and academic partners, ORNL researchers are using simulations and modeling to determine safe, efficient ways to improve energy production from nuclear reactors.

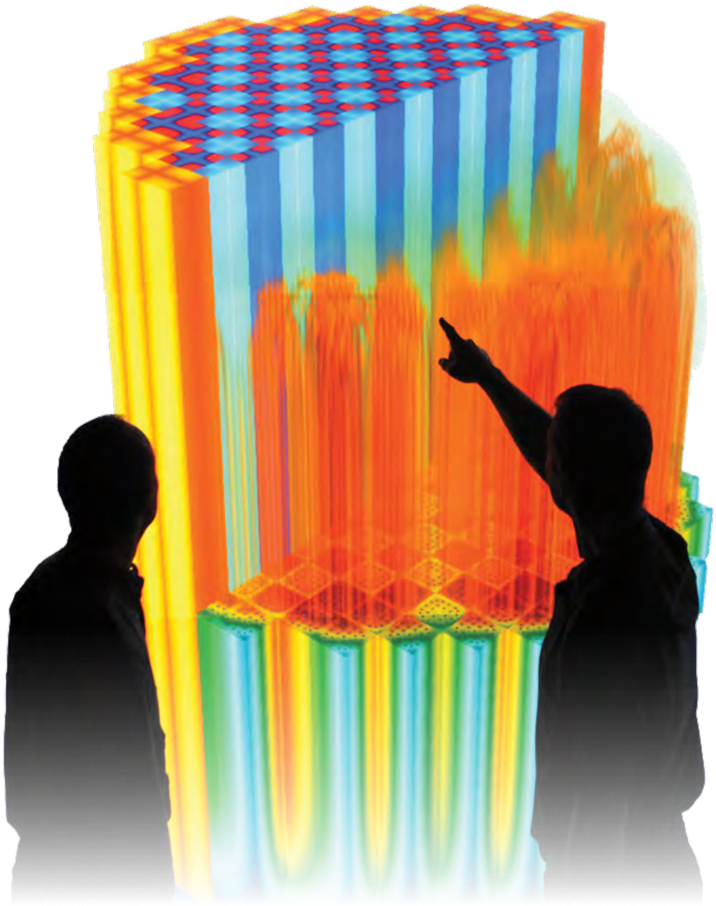
ORNL's leadership in nuclear science and technology is essential for ensuring a safe, effective nuclear infrastructure today, while paving the way for tomorrow's nuclear breakthroughs.



ITER is being built to demonstrate the feasibility of industrial-scale fusion energy.



Tennessee Valley Authority's Watts Bar Nuclear Plant



Isotopes for medicine, industry, and research

ORNL's High Flux Isotope Reactor, constructed in the 1960s to produce transuranic isotopes, is still the western world's sole supplier of californium-252, an isotope instrumental in the exploration of new energy resources, medical therapy, and the detection of pollutants in the environment and explosives in luggage.

Improving reactor performance

New nuclear power plant technologies are expensive to test, and new plants cost billions to construct. ORNL is helping address these challenges as host of a DOE-sponsored partnership of government, academia, and industry called the Consortium for Advanced Simulation of Light Water Reactors (CASL). CASL is using the lab's supercomputers and advanced modeling and simulation techniques (pictured at left) to figure out how to safely extend the life of reactors and implement new technology that's safer, more efficient, and more reliable.

ORNL Capabilities Vital to Nuclear Science & Technology

Accelerator science • Advanced computer science, visualization, and data • Applied materials science and engineering • Applied nuclear science and technology Chemical and molecular science • Chemical engineering • Computational science • Condensed matter physics and materials science • Large-scale user facilities/advanced instrumentation • Nuclear physics • Plasma and fusion energy sciences • Systems engineering and integration

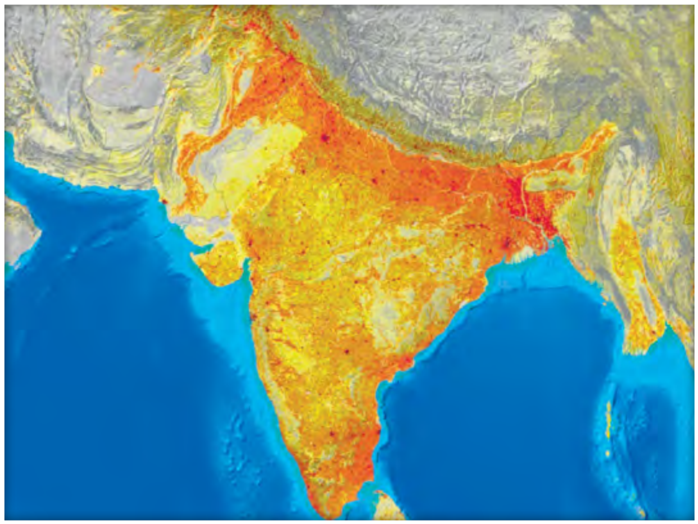
Establishing partnerships, spurring economic development

ORNL promotes an entrepreneurial culture that puts science to work through licensing of its intellectual property and application of its expertise to the challenges facing private industry.

The lab has more than 140 active licenses with organizations ranging from startups to large corporations to academic institutions. The innovation of ORNL researchers results in more than 200 inventions and an average of 50 patents each year. ORNL has won more R&D Awards, given by *R&D Magazine* for the top 100 inventions each year, than any other organization.

Businesses come to ORNL for assistance solving difficult technical problems or finding better ways to do their work. The resulting scientific partnerships allow lab innovations to reach the private sector, promoting commercialization and job growth.

LandScan™



The LandScan High Resolution Global Population DataSet, developed at ORNL, refines the best available census data using geographic information system and remote sensing technologies and has emerged as an international community standard for sustainable development, environmental protection, disaster response, and humanitarian relief.

Manufacturing stronger, lighter material

The Oak Ridge Carbon Fiber Composites Consortium includes more than 40 companies seeking to develop new, low-cost materials and processes that will greatly accelerate the commercial use of carbon fiber and composites in applications including transportation, aerospace, wind and alternative energy, oil and offshore drilling, and construction. The lab's Carbon Fiber Technology Facility can produce up to 25 tons of material annually as researchers and industry partners seek to efficiently produce the strong, lightweight material at a commercial scale.

Partnerships with private companies, universities, nonprofit agencies, and other nonfederal entities are made possible through a variety of mechanisms, including cooperative research and development agreements, work-for-others contracts, user agreements, and nondisclosure agreements.

By promoting the creation and expansion of technology-based companies and better-paying jobs, ORNL is a significant economic-development resource, improving the quality of life in the region, state, and nation.

Training tomorrow's scientific leaders

ORNL links university students and faculty across the United States with multidisciplinary research opportunities and unique facilities, bringing outstanding future scientists, engineers, and teachers together with today's finest researchers. More than 1,000 students conduct research at ORNL each summer.

The University Partnerships Program provides graduate internships and fellowships, postdoctoral appointments, joint faculty positions, and collaborative research. Students also get one-of-a-kind entrepreneurial experience through opportunities such as development of business plans for technology deployment. ORNL's vision is to transform the graduate educational experience by engaging students in large-scale, problem-oriented programs that enable scientific discoveries and innovative solutions to energy-related challenges.

Bredesen Center for Interdisciplinary Research and Graduate Education

The Bredesen Center for Interdisciplinary Research and Graduate Education (CIRE) offers exceptional doctoral fellowships. Extensive interdisciplinary research and coursework focus on science and engineering challenges related to the production, distribution, and consumption of energy. Students also gain skills and experience in public policy and entrepreneurship, joining research teams at ORNL and the University of Tennessee in problem-oriented research.

ORNL researchers talk to graduate students during the CIRE speed networking event, a round-robin-style interaction that allows students to meet as many research staff members as possible in a brief timespan and includes poster presentations by Bredesen Center students.

UT-Battelle's Core Partners

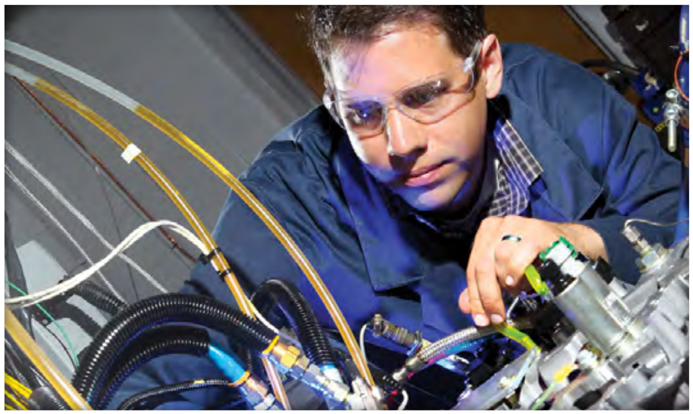
Attracting researchers from around the globe

The accelerator-based **Spallation Neutron Source** provides the most intense pulsed neutron beams in the world, revealing details about extraordinarily small samples of physical and biological material.

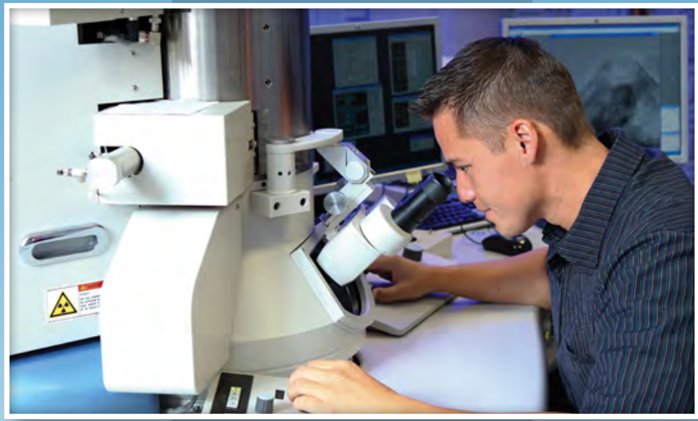
The **Center for Nanophase Materials Sciences** integrates nanoscale science with theory, modeling, and simulation for a better understanding of subatomic systems and architectures with the potential to revolutionize technology.

The 85-megawatt **High Flux Isotope Reactor** has one of the highest steady-state neutron fluxes in the world, allowing scientists to study the molecular and magnetic behaviors of materials. It also is a key facility for isotope production, neutron irradiation, and neutron activation analysis.

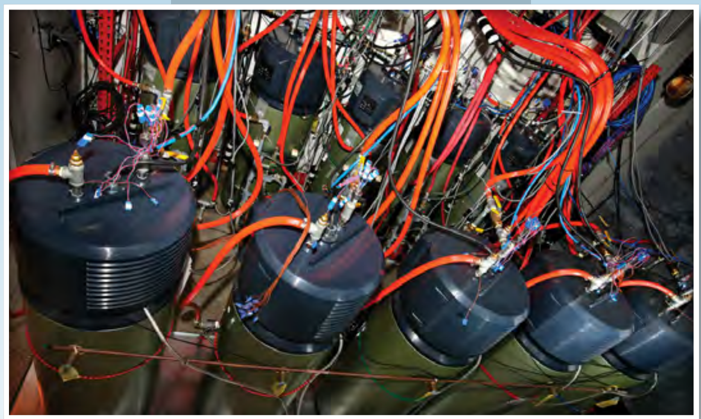
The **Oak Ridge Leadership Computing Facility** offers some of the world's most powerful supercomputers. From astrophysics to combustion to fusion and dozens more areas across the scientific spectrum, the center's simulations make transformational break-throughs possible at lower cost and in less time.



The **National Transportation Research Center** helps industry, academia, and other agencies advance technologies that improve fuel economy, reduce emissions, and address issues such as traffic congestion, evacuation planning, and highway safety.



The **Shared Research Equipment User Facility** is an electron beam microcharacterization facility that provides a suite of advanced instruments for micrometer- to angstrom-scale characterization of materials.



The **Building Technologies Research and Integration Center** offers a wealth of experimental and computational tools and expertise on building envelopes; equipment and fluids for heating, cooling, and appliances; and system and whole-building performance to support development and performance characterization of technologies that maximize the cost-effective energy efficiency of residential and commercial buildings.

Integrating expertise across the scientific spectrum

Accelerator Science and Technology

ORNL's expertise includes the physics and supporting technology for production, acceleration, accumulation, and use of high-intensity, high-power beams of atomic particles.

Advanced Computer Science, Visualization, and Data

ORNL's computational capability includes experts in system software, component technologies, architecture-aware algorithms, fault-tolerant distributed computing, virtualization, computational steering, networking, data analytics, and cybersecurity.

Applied Materials Science and Engineering

ORNL researchers apply knowledge of materials characterization, synthesis, processing, and design to applications such as advanced manufacturing and creation of lightweight materials, advanced steels and coatings, nuclear fuels and structural materials, batteries, solar photovoltaics, and materials for extreme environments.

Applied Nuclear Science and Technology

ORNL advances reactor and fuel-cycle technology; addresses challenges in nuclear nonproliferation, national security, and environmental management; and supports isotope production and R&D. Scientists also use modeling and simulation to advance understanding of the fuel cycle and improve the efficiency and use of nuclear systems and associated experimental facilities.

Biological Systems Science

ORNL scientists in plant molecular biology and microbiology develop and apply advanced capabilities to solve problems in bioenergy, climate change, carbon sequestration, and the health effects of low-dose radiation. As the lead institution for DOE's BioEnergy Science Center, ORNL is pioneering systems biology science, leading to economical and sustainable production of biomass material and its conversion to biofuels and other products.

Chemical and Molecular Science

ORNL's capabilities encompass design, synthesis, and characterization of the structure and reactivity of organic, inorganic, biological, polymeric, and hybrid materials. A particular strength at ORNL is understanding and controlling the chemistry at interfaces between phases of materials (e.g., liquid and solid).

Chemical Engineering

ORNL applies knowledge supplied by fundamental chemical research to efforts including nuclear fuel reprocessing and isotope production and separation as well as energy efficiency, renewable energy, fossil energy, waste management and environmental remediation, and national security.

Climate Change Science

ORNL addresses the implications of climate change at scales from local to global and leads fundamental studies of climate change impacts on the terrestrial carbon and other biogeochemical cycles as well as their connections to other natural and human systems.

Computational Science

ORNL is the world's most capable complex for computational science as a result of its staff, infrastructure, and high-performance computing systems. A distinctive feature of this core capability is the ability to build multidisciplinary teams to execute breakthrough science through scalable algorithms and codes on massively parallel hardware.

Condensed Matter Physics and Materials Science

ORNL's research focuses on understanding multiscale physical and chemical phenomena that underpin the discovery of advanced materials, with the goal of enabling new technologies for energy production, storage, and use.

Environmental Subsurface Science

ORNL capabilities in environmental subsurface science are advancing the fundamental understanding of contaminant transport and transformation in natural environments and enabling solutions to subsurface contamination by uranium and nitrate and surface contamination by mercury.

Large-Scale User Facilities/Advanced Instrumentation

ORNL has a distinguished record in the design, procurement, construction, and operation of major facilities for DOE and in the development of advanced instrumentation for acquisition, management, analysis, and visualization of experimental data. These facilities have innovative instrumentation and research programs that serve to motivate and attract users.

Nuclear Physics

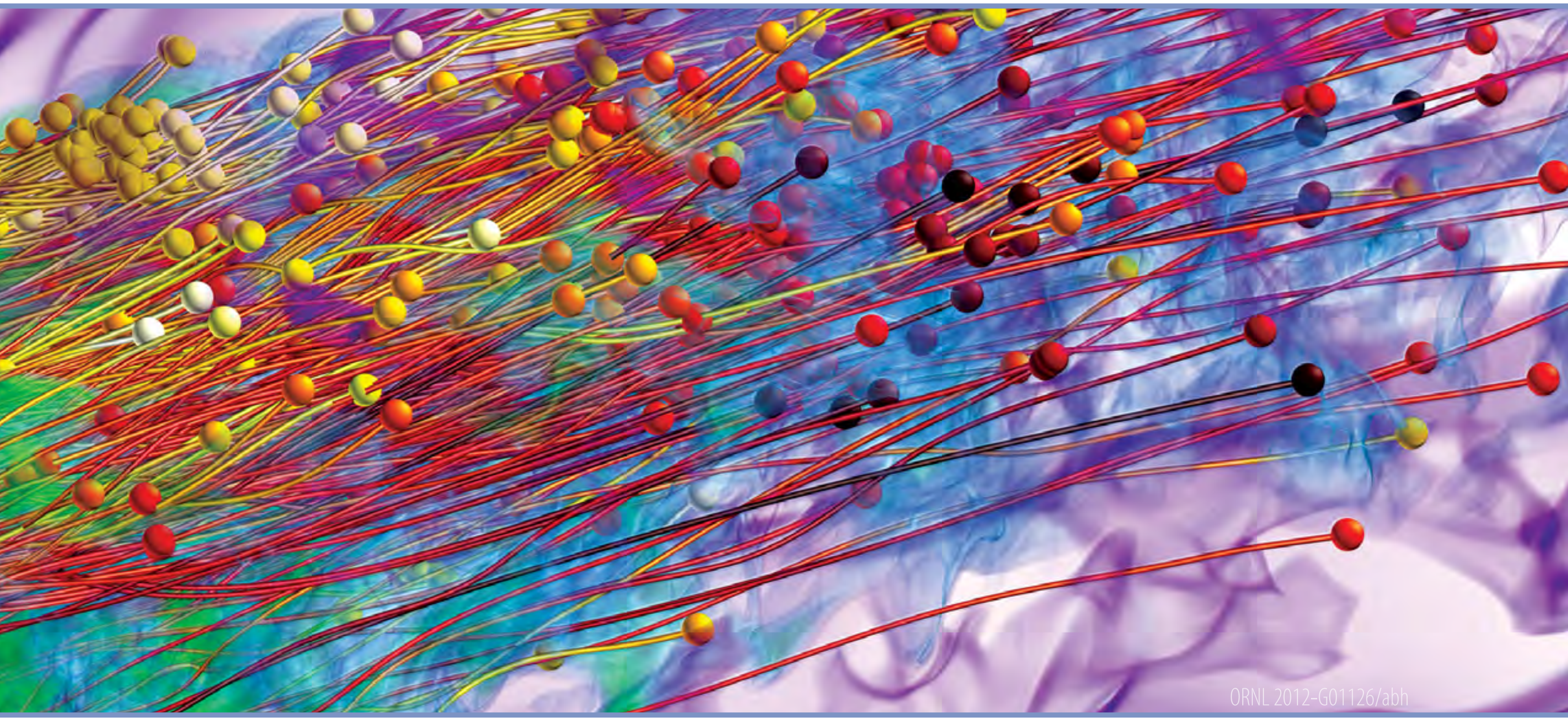
ORNL's nuclear physics capability includes theoretical, experimental, and simulations expertise. Research by ORNL nuclear physicists expands our understanding of the structure and origin of nuclei and advances physics beyond the Standard Model.

Plasma and Fusion Energy Sciences

ORNL leads US contributions to the international effort to harness fusion energy and conducts research in fusion plasma physics, materials, and fusion technology.

Systems Engineering and Integration

ORNL has a reputation for creating large, complex, one-of-a-kind systems that must be field-deployable, maintainable, and reliable. Repeated success with high-risk, nationally important projects has created a unique ability to deliver such systems.



Oak Ridge National Laboratory's mission is to deliver scientific discoveries and technical breakthroughs that will accelerate the development and deployment of solutions in clean energy and global security, and in doing so create economic opportunity for the nation.

UT-BATTELLE

U.S. DEPARTMENT OF ENERGY | Office of Science