







# SCIENCE ALLIANCE 2012-13 CREATING OPPORTUNITY

THE UNIVERSITY OF TENNESSEE KNOXVILLE













# CREATING OPPORTUNITY



## From the Director

The Science Alliance continues to support collaborative research between the faculty at the University of Tennessee, Knoxville, and the scientific communities at the Oak Ridge National Laboratory.

Nowhere is this collaboration more prominent and important than in the Joint Faculty programs that have been set up between our two institutions. In this year's annual report we present a brief overview of the different types of joint faculty that have developed over the years.

Many of you have probably heard of the Distinguished Scientist and Governor's Chair programs—the standard bearers for identifying and "growing" areas of collaboration between the national laboratory and university. However, other kinds of collaborative appointments existed between the two institutions before the Distinguished Scientist and Governor's Chair programs were initiated, and currently additional types of joint appointments exist as well.

One of the areas of science that is a natural for collaboration between scientists at ORNL and faculty members at UT is neutron science. The decision by the US Department of Energy to build the world's most powerful Spallation Neutron Source at ORNL made it a likely focus for collaboration in engineering and the sciences. The list of experiments possible at the SNS is now ramping up to a full head of steam as more and more experimental stations come on line and the neutron flux is ever higher. A second feature article describes some of the unique advantages of using neutrons to probe the properties of matter.

Finally, we would like to announce and congratulate the recipients of the Science Alliance Joint Directed Research and Development awards for 2013. As we have in the past, a brief sketch of the research that these awards support is provided.

Craig & Barnes

# Accelerator physics. Gas hydrates. Spallation neutron science.

Without the UT-ORNL Joint Faculty program, these terms probably wouldn't be commonplace at the University of Tennessee.

BY LUCINDA HODGE

A collaboration established between UT and the Oak Ridge National Laboratory, the Joint Faculty program opens unique avenues of research for both institutions and provides numerous benefits to each.

"The Joint Faculty program allows one to build a large and focused university-based research group while also having access to the broad technical expertise and world-leading facilities of a top national laboratory," said Jimmy Mays, a UT-ORNL Distinguished Scientist and professor of chemistry. "This synergistic relationship boosts productivity and the impact of the science."

Currently, there are three types of joint faculty at the university. The first type consists of Distinguished Scientist and Governor's Chair level appointments. The appointments are made with the expectation that these individuals will help lead research efforts at both institutions in their fields of specialization.

According to Hanno Weitering, professor and Head of UT's Department of Astronomy and Physics, the second type normally has a 50 percent appointment at UT. Faculty on this appointment teach, submit proposals through the department, obtain research funding, and supervise students.

Approximately 102 scientists at ORNL hold a third type of appointment at UT called the zero percent appointment. These typically come about when an ORNL scientist has a close collaborative research connection to one or more faculty members in a department.

According to Lee Riedinger, a professor of physics and director of UT's Bredesen Center for Interdisciplinary Research and Graduate Education, the zero percent program is part of a long history of collaboration between UT and ORNL.

In the '60s, a Ford Foundation grant set up a pool of money that enabled Oak Ridge faculty to come to the university for a one-day appointment. When the award ran out, university departments took over the funding for several years.

In 1999, as a result of state funding awarded by Tennessee Governor Don Sundquist, UT began hiring more collaborating scientists, which it labeled joint faculty.

"It was basically a loan employee agreement," Riedinger says. "They decided the shared employee mechanism was the right way to go. That opened the floodgates."

Riedinger says the US Department of Energy and ORNL allow joint faculty to be set up at zero percent time at the university, which gives them the opportunity to have full rights to be real mentors to UT students and the students the benefit of easier access to ORNL's world-class instrumentation. While zero percenters don't enjoy all the benefits full-time university faculty do, this appointment provides Oak Ridge faculty access to funding with agencies such as the National Science Foundation and National Institutes of Health.

"Zero percent appointments represent a more substantial partnership, in my view, than adjunct appointments because they require more work to set up, including the involvement of the division director," Riedinger says.

Claudia Rawn, now the director of UT Center for Materials Processing, represents an interesting example of how a joint appointment can "evolve" over time.

Rawn joined the Materials Science and Technology Division at ORNL in 1997 with the Oak Ridge Associated Universities Postdoctoral Fellowship program. When she was hired into the Joint Faculty program in January 2002, she held a 60 percent ORNL and 40 percent UT appointment and began to bring her research program in gas hydrates to the university.

In January 2012, her appointment changed to 80 percent UT and 20 percent ORNL, and she became the associate director of the Center for Materials Processing. Six months later, she became the director, and in January 2013, her joint faculty appointment was changed to 90 percent UT and 10 percent ORNL.

Rawn says collaboration is an important mutual benefit of the Joint Faculty program. Knowing people at both institutions, she can recommend qualified students for positions with her colleagues at ORNL. If she's writing a grant proposal, she knows which ORNL colleagues can provide the best information for the project.

Rawn's specialty at ORNL is using X-ray and neutron scattering techniques to characterize a variety of materials. At UT, her students use a range of techniques to synthesize materials. Then they characterize the material at one of the DOE User Facilities at ORNL, including the Spallation Neutron Source, High Flux Isotope Reactor, and Center for Nanophase Materials Sciences. To gain access the students must write competitive proposals for "beam time." If approved they take general safety and instrument-specific training before using the instruments. Once there, they load the samples, collect data for some number of days, and then analyze the data and results. They are able to spend time with the various beam line scientists who are experts in their field and often present their research at technical meetings and write co-authored manuscripts.

"Being able to open that door to my students has been very beneficial," Rawn says.

Weitering says zero percenters are making a positive impact, for instance, by bringing research in accelerator physics to the department and also through their work with students.

Jeremy Smith, the university's first Governor's Chair and also director of the UT-ORNL Center for Molecular Biophysics at ORNL, says all his research depends on the Joint Faculty program. Smith also indicated all of his bioenergy projects involve others at the university. In return, UT has access to the world-class facilities at ORNL.

Smith, whose wide range of research topics include bioenergy, supercomputing, and drug design, says the UT-ORNL partnership is vital to the university's quest to become a Top 25 public research university.

"Collaboration with ORNL is absolutely essential if UT wants to make the Top 25," Smith says. "ORNL is number one in the world in what it does."

Joint faculty collaboration also helps with student recruitment and retainment

"A lot of students have heard of Oak Ridge National Laboratory, so just knowing that the two have strong collaborations and there are chances for students to go out there and use some of the equipment and network with the ORNL researchers definitely helps with recruitment," Rawn says.

"Joint faculty also work with undergraduate students at ORNL during the summer. Some of those students may decide to stay at UT for graduate school," Weitering says.

Rawn says the Joint Faculty program is run smoothly.

"I think it works great. UT is a much older institution than ORNL. It just seems that academics in general have a pretty good support system, and I appreciate that."

Smith agrees. "It's fun doing all these scientific projects, working with talented people and bright researchers at ORNL. It's the future of UT."





# **Cong Trinh**Single-Cell Diesel Production

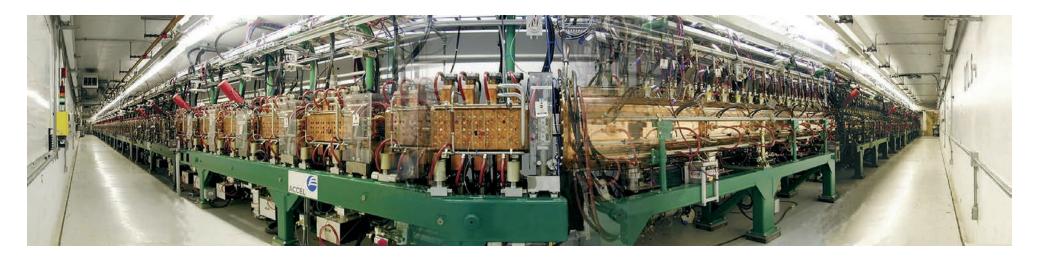
It hasn't been that long ago that the idea of designing individual biodiesel producing yeast or bacteria cells would have seemed like a pipedream. But today, advanced genetic and microbial engineering tools are changing science-fiction pipedreams to science.

Single cell production, as it is called, intrigues Cong Trinh and ORNL's Adam Guss. The two have joined forces to find out what it would take to turn common yeast, *S. cerevisiae*, and *E. Coli* into miniature cell factories that directly convert the fermentable sugars, lignin, and the chemical inhibitors found in biomass into an array of advanced biofuels and other biochemicals.











# David Keffer I Experiment, Therefore I Compute

Experimentation and computation are inextricably linked in many if not most research projects of our time. But what is critical to success—and far less obvious—is how essential communication becomes among members of an interdisciplinary team who engage in this joint enterprise. Number-crunching modelers can only simulate and accurately compare data if they understand the experimentation of their colleagues.

David Keffer and his computational team provide experimentalists at ORNL with proven, molecular-level guidance to understanding the fundamental relationship between nanostructure and lithium-ion conductivity in new carbonfiber anodes that will transform battery technology.







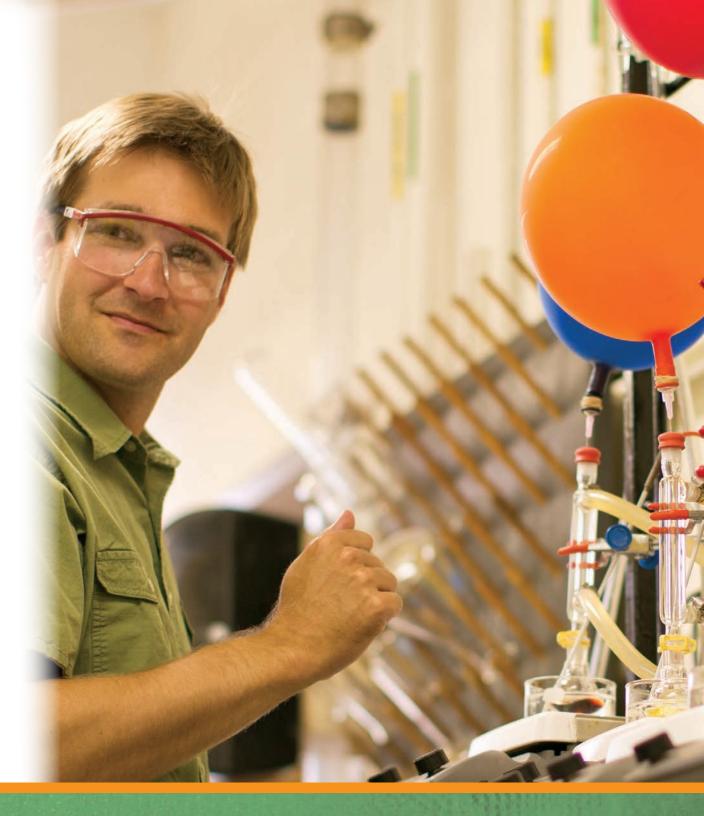
# **David Jenkins**Capture and Release

In 2010, the Environmental Protection Agency reported that 55 percent of all greenhouse gas emissions in the US came from industry—much of it released into the atmosphere in flue gas.

Currently, removal technology wet scrubs the gas with ammonia compounds, but we pay a high-energy penalty to regenerate and reuse the volatile and corrosive scrubbing solutions.

David Jenkins and a team led by ORNL's Radu Custelcean are pursuing an alternative technology designed to strip carbon dioxide from flue gas by forcing it through dry, porous microcrystals that attract and hold CO2 until it can be released without entering the atmosphere.





# **Edmund Perfect**

Thaw. Freeze. Repeat.

Even in our home kitchens—where we keep a small chunk of the Ice Age in a box—we all know it is not a good thing when the refrigerator freezer thaws, and our frozen items melt. The food spoils.

How much greater the consequences for entire Arctic landscapes where thawing of permanently frozen ground (permafrost) is occurring on a massive scale due to climate change.

The collaboration led by Ed Perfect and ORNL's Richard Mills pairs a profound knowledge of the physical processes involved in ground freezing and thawing with supercomputing to model the impacts of global warming.





# Tongye Shen Probing Protein

Genes may get all the glory, but proteins are where the action is.

Our ability to understand the dynamic motions of proteins is what really counts when we peer into biological systems and observe how they respond to change. Increasingly complex studies of protein systems—as they change shapes to regulate and signal biological processes—hold enormous promise for advances on many research fronts.

In collaboration with ORNL scientists using world-class neutron technology and supercomputing facilities, Tongye Shen targets the challenge of studying complex protein systems with a powerful combination of modeling, theoretical, and computational tools.



# Veerle Keppens Reclaiming Energy

US Department of Energy studies show only 14 to 26 percent of the energy from the fuel in your gas tank moves your car down the road. Sixty to 70 percent is lost as heat.

Materials that generate electricity from waste heat or provide cooling when a current is passed from one side to the other (thermoelectrics) offer one possibility for recovering some of this energy. But, efficient thermoelectric materials require the unusual combination of poor thermal conductivity and good electrical conductivity.

Working in tandem, Veerle Keppens and ORNL's Olivier Delaire search for microscopic clues to the origins of suppressed thermal conductivity in hopes of finding useful new thermoelectric materials.







# **Eric Lukosi**

# Finding Without Fail

Failures of nuclear and storage facilities at Fukushima Daiichi and Yucca Mountain highlight the importance of containment materials as a first line of defense for preventing the release of nuclear fission products.

Neutron imaging is an ideal diagnostic tool for evaluating the structural integrity of those materials, with implications for safety, shipping, and long-term storage.

Eric Lukosi takes the first step in the long road toward achieving a next-generation neutronimaging sensor that will be able to characterize and confirm whether the materials we choose to use in critical applications remain effective and safe.



# Andy Sarles Naturally Inspired

Cell membranes teach us about "how things work" in the natural world.

Painstaking research decodes the membrane's complex, interacting proteins, peptides, and enzymes. What researchers learn often inspires practical biomolecular tools or brings clarity about diseases, Andy Sarles says.

Sarles and his ORNL counterpart, Shuo Qian, want to know if a relationship exists between cholesterol in the cell membrane and the plaque-forming amyloid beta fibrils linked to debilitating Alzheimer's disease.

Sarles' team uses a tool invented to create artificial cell membranes between two water droplets. With it they can control membrane composition, size, and other properties—historically a difficult task to accomplish.



# **Spallation Neutron Source**

# Seeing is Believing

Remember the old saying, "see no evil, hear no evil, speak no evil"? This prototypical perspective of polite, civilized society gets turned on its head in science and engineering. Ideally, researchers want to see, hear, and speak it all—both at a human scale and at scales that match the phenomena under investigation—in a time frame of their own choosing.

Then they want to make sense of it all as quickly as possible, tell the world what they've found, and move on to the next question.

Here in East Tennessee we are fortunate to live at a time and in a place where one of the largest and finest facilities for sensing and seeing finds its home.

## **The Spallation Neutron Source**

Since 2006, the immense Spallation Neutron Source (SNS) facility at ORNL has lit a fire under scores of new ventures in neutron technology and custom instrument design.

This accelerator-based facility provides the most intense pulsed neutron beams in the world for scientific research and industrial development. Each year, it hosts hundreds of researchers from universities, national laboratories, and industry, who conduct basic and applied research and development using neutrons.

With the presence of this invaluable laboratory facility on our home turf, it

BY THERESA PEPIN & LAURA BUENNING

is worth the time to learn more about neutrons and their use in experiments that probe and peer into all kinds of samples.

## Why Neutrons?

In contrast with more familiar X-rays, whose imaging is based on material density, neutrons reveal structure and function based on the different elements in a material. X-ray (photon) and electron beams interact with electrons, while neutrons interact primarily with atomic nuclei.

Neutrons are non-invasive and non-destructive probes; they can deeply penetrate but do not damage samples; they can precisely locate "lighter" atoms such as hydrogen or oxygen, for example, among "heavy" atoms such as mercury or other metals; they can track molecular vibrations and movements of a protein; they are impervious to extreme environmental conditions and have both particle- and wave-like properties.

Upon penetration of a given sample, the neutrons' particle/wave properties make it possible to use a technique called neutron scattering whereby scientists count scattered neutrons, measure their energies and the angles at which they scatter, and map their final positions. Neutrons can also be used to create two- and three-dimensional images of the distribution of light elements in a material (known as neutron imaging).

Taken together these methods can reveal the structure and behavior of materials over multiple scales.

Neutron technology is a powerful cutting-edge technique in the arsenal of scientific tools needed to probe materials and understand the full range of structural properties.

JDRD researchers seek to see—accurately and productively—in a wide range of ways, over scales never before imagined. Joint Directed Research and Development funding allows them to take that challenge to a new level.



## Governor's Chairs

The Governor's Chair program attracts exceptionally talented, internationally recognized research scientists and engineers to joint appointments as tenured UT professors and ORNL distinguished research staff. Initiated by former Tennessee Governor Phil Bredesen, the program takes advantage of the synergy between the state's flagship campus and the nation's leading multipurpose national lab. The program is managed through the UT Office of the Executive Vice President.

## Sudarsanam Suresh Babu Advanced manufacturing

UT Departments of Mechanical, Aerospace & Biomedical Engineering and Materials Science & Engineering; ORNL Energy and Environmental Sciences Directorate, Energy Material Program

Sudarsanam Suresh Babu hones advanced manufacturing processes, including additive techniques, also know as 3-D printing, which adds successive layers to make a three-dimensional solid object from a digital model. His work emphasizes energy-efficient design and development, product life cycles and the implications of design on the product's purpose.

#### Howard Hall Global nuclear security

#### UT Department of Nuclear Engineering; ORNL Division of Global Nuclear Security Technology

Howard Hall applies his background in nuclear chemistry to the nearly overwhelming challenges in nuclear security. His research addresses questions of proliferation, counter-proliferation, detection of and response to radiological or nuclear threats, radiochemistry, and nuclear forensics.

# **Terry Hazen**Environmental microbiologists; Bioremediation and bioenergy

#### UT Departments of Civil & Environmental Engineering, Microbiology, and Earth & Planetary Sciences; ORNL Division of Biosciences

Terry Hazen studies what happens as naturally occurring bacteria break down and detoxify hazardous materials, such as metals/radionuclides, petroleum, and chlorinated solvents. His group explores environmental biogeochemical stress-response pathways, from the molecular to the ecosystem level.

#### Yilu Liu

#### Power systems and smart-grid technology

#### UT Department of Electrical Engineering and Computer Science; ORNL Division of Energy and Transportation Science

Yilu Liu develops new and better ways to monitor and understand flow of electricity through the nation's power grid. Her group is working to devise a smarter electric grid that automatically resolves minor disruptions before they escalate to major blackouts.

# Frank Loeffler Environmental systems microbiology

# UT Departments of Microbiology and Civil & Environmental Engineering; ORNL Division of Biosciences

Frank Loeffler's research team characterizes the intricate microbial processes that enable naturally occurring bacteria to break down toxic contaminants, immobilize radioactive wastes, reduce greenhouse gas emissions, and control the biogeochemical cycling of carbon and nitrogen in soils, sediments, and freshwater bodies, including groundwater.

## Ramamoorthy Ramesh Nanomaterials engineering

# UT Department of Materials Science & Engineering; ORNL Deputy Director for Science and Technology

Ramamoorthy Ramesh is internationally recognized for his work on complex multifunctional oxide thin films, nanostructures, and heterostructures. His published research ranges from magnetic materials to high-temperature superconductors to advanced transmission electron microscopy techniques applied to materials characterization.

# Jeremy Smith Molecular biophysics simulation

# UT Department of Biochemistry & Cellular & Molecular Biology; ORNL Division of Biosciences

Jeremy Smith and the Center for Molecular Biophysics team of UT professors and ORNL staff scientists combine experimental neutron scattering and large-scale computational simulation and modeling techniques to describe molecular structure and motion.

# Alexei Sokolov Dynamics of soft materials

#### UT Departments of Chemistry and Physics & Astronomy; ORNL Division of Chemical Sciences

Alexei Sokolov studies molecular motion as the key to macroscopic properties of materials. His primary interest is in the fundamental properties of soft materials—or by definition, materials that can change.

## William Weber Materials' response to radiation

# UT Department of Materials Science & Engineering; ORNL Division of Materials Science and Technology

William (Bill) Weber's team uses direct measurements of materials irradiated with high energy ions in UT's new particle accelerator and powerful computational simulation to predict the long-term resilience of materials in nuclear environments.

# Robert W. Williams Genetics and human health

# UT Health Science Center, Department of Anatomy and Neurobiology

Robert (Rob) Williams studies genetic and environmental causes of human diseases using novel mouse populations and massive human genetic data sets. His group's research ranges from metabolic to neuropsychiatric diseases.

# **Brian Wirth**Computational nuclear engineering

#### UT Department of Nuclear Engineering; ORNL Consortium for Advanced Simulation of Light Water Reactors

Brian Wirth investigates the performance of nuclear fuels and structural materials in nuclear environments. His research improves predictions about the longevity of nuclear reactor components.

# Thomas Zawodzinski Electrical energy storage

#### UT Department of Chemical and Biomolecular Engineering; ORNL Division of Materials Science and Technology

Thomas (Tom) Zawodzinski explores basic mechanisms of chemical processes occurring in materials found in electrochemical systems, such as batteries and fuel cells. His team characterizes and improves the rates of those all-important chemical reactions at the heart of fuel cell and battery technology.

## Distinguished Scientists

The Distinguished Scientist Program supports high-profile, internationally recognized leadership appointments in science and engineering. The program anchored the Science Alliance partnership-building role during the center's early years. Appointees were recruited to joint UT-ORNL positions as tenured distinguished UT professors and senior ORNL research staff. Since 2005, joint appointments at this level have been made through the Governor's Chair Program.

## **Elbio Dagotto**

## Nanoscale dimensions and correlated electronic behavior

#### UT Department of Physics & Astronomy; ORNL Division of Materials Science and Technology

Elbio Dagotto primarily uses computational techniques to study transition metal oxides, oxide interfaces, and the recently discovered iron-based, high-temperature superconductors. These materials and others studied by his group show promise both for technological applications and for advancing fundamental concepts in condensed matter physics.

## Takeshi Egami

# Atomic-scale dynamics of liquids and glasses; High-temperature superconductivity

# UT Departments of Materials Science & Engineering and Physics & Astronomy; ORNL Division of Materials Science and Technology

The physics of liquids and glasses is much less developed than the physics of crystalline solids. Takeshi Egami explores new science of liquids and glasses using computer simulation, including quantum mechanical calculations, and neutron and synchrotron x-ray scattering experiments.

# **Georges Guiochon Separation science**

#### **UT** Department of Chemistry

Georges Guiochon is an expert in using multidimensional chromatography to separate the components of complex samples. His research improves the efficiency of chromatographic columns, optimizes conditions for maximum production rate of safe and effective pharmaceuticals, and examines the complex fundamentals of supercritical fluid chromatography.

#### Robert Hatcher Structural geology and tectonics of continental crust

#### **UT Department of Earth and Planetary Sciences**

A structural and tectonics geologist, Bob Hatcher studies the processes that create and evolve Earth's continental crust.

# **David Joy**Accurate microscopic and nanoscale imaging

Science and Technology

#### UT Departments of Biochemistry & Cellular & Molecular Biology and Materials Science & Engineering; ORNL Division of Materials

David Joy's research helps create accurate microscopic and nanoscale imaging techniques, including the new, superior-performing Helium lon Beam microscope, which is more flexible and powerful than electron microscopy and ultimately could offer direct, high-resolution imaging at subatomic and subnanometric scales.

# Joseph Macek Electron vortices in simple atomic systems

#### **UT Department of Physics & Astronomy**

The probabilities of finding electrons at given points in space are described mathematically in quantum mechanics. Joseph Macek relies on this theory to study what happens to simple, fragmented atomic systems when atoms collide.

#### Jimmy Mays Synthesizing new polymer membranes for fuel cells

#### UT Department of Chemistry; ORNL Division of Chemical Sciences

Jimmy Mays synthesizes new, precisely tailored polymers and examines their molecular architecture, composition, and blending capability to discover how form and structure, including their nanostructural order, might be manipulated to create useful materials.

## **UT-ORNL** Joint Institutes

Five UT-ORNL joint institutes link distinct, complementary resources in select, high-priority scientific and engineering fields at The University of Tennessee, Knoxville, and Oak Ridge National Laboratory. Each opens doors to leadership-class research instrumentation and computing facilities; offers an environment conducive to collaboration; and provides the physical space where scientists and engineers can exchange ideas and work collectively to answer complex research questions.

#### **UT-ORNL Joint Institute for Advanced Materials**

The Joint Institute for Advanced Materials (JIAM) promotes interdisciplinary research and education related to developing new materials with superior properties (such as greater toughness and high-temperature strength) or those that can be tailored to support new technologies (such as pocket-sized supercomputers).

## **UT-ORNL Joint Institute for Biological Sciences**

The Joint Institute for Biological Sciences (JIBS) supports interdisciplinary, crosscutting research that accelerates progress in complex bioenergy and bioenvironmental systems. It also aids access by UT-ORNL faculty, staff, and students to state-of-the-art capability in genomic, transcriptomic, proteomic, and metabolomic analysis of biological and environmental systems.

## **UT-ORNL Joint Institute for Computational Sciences**

The Joint Institute for Computational Sciences (JICS) advances scientific discovery and state-of-the-art engineering and computational modeling and simulation. JICS takes full advantage of the petascale and beyond computers in the Department of Energy National Center for Computational Sciences (NCCS) and UT's National Institute for Computational Sciences (NICS).

#### **UT-ORNL Joint Institute of Nuclear Physics and Applications**

The Joint Institute of Nuclear Physics and Applications (JINPA) links UT, ORNL, and Vanderbilt University research that explores the structure of atomic nuclei, via several types of experimental programs and an extensive UT-ORNL theoretical nuclear physics initiative.

#### **UT-ORNL Joint Institute for Neutron Sciences**

The Joint Institute for Neutron Sciences (JINS) promotes worldwide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences.







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