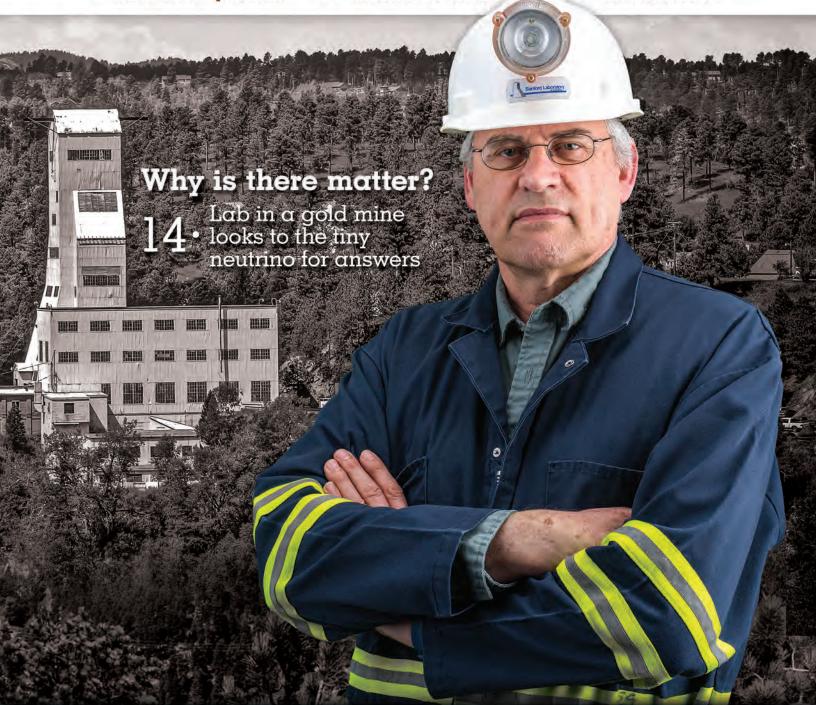
OAK RIDGE NATIONAL LABORATORY

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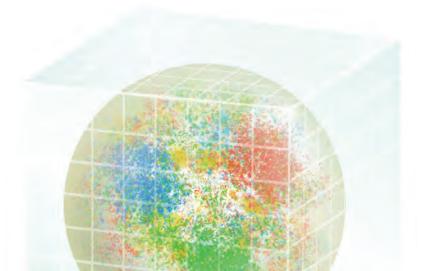
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On the Cover

ORNL physicist David Radford is using the tiny neutrino to address big questions with an experiment housed at a retired gold mine in South Dakota.



ORNL is fundamentally strong

ORNL has always been a great place for people exploring big questions.

Whether you're a physicist, a chemist, a materials scientist or the kind of eclectic researcher who's hard to nail down, the lab provides the resources and environment that encourage pursuit of important answers.

In the first place, we value collaboration. Our team approach applies diverse expertise to science's most difficult problems, tapping assets across the lab and in academia and industry.

ORNL offers an array of unique and powerful research tools, including two of the world's leading neutron facilities (page 11), a diverse collection of microscopes and other instruments for analyzing material atom by atom (page 9), and the nation's most powerful supercomputer (page 7).

In this issue of *ORNL Review*, we focus on efforts to understand the workings of the universe, from its earliest moments to its tiniest particles.

Occasionally this work takes our staff off-site. Physicist David Radford co-leads the Majorana Demonstrator, a lab nearly a mile deep in a retired gold mine in South Dakota that could help explain why the universe has more matter than anti-

matter (page 14). In Europe, physicist Tom Cormier leads the American contribution to the ALICE experiment at the Large Hadron Collider. ALICE collides lead nuclei at nearly the speed of light to create quark-gluon plasmas, a state of matter largely unseen since a millionth of a second after the Big Bang (page 20).

Quarks and gluons are held together by the strong force, one of the universe's four fundamental forces. In this issue, you can read about efforts to use Titan to advance the study of the strong force, called quantum chromodynamics (page 22). Titan is also helping to analyze a mountain of cancer data to improve treatments (page 18).

Quantum materials governed by the interactions amongst atoms and electrons can have astonishing—and astonishingly useful—properties. We look at ORNL research into these remarkable materials (page 24), including projects focused on specific materials such as superconductors (page 6) and quantum spin liquids (page 12).

As always, this issue introduces you to noteworthy scientists, both established in their careers (pages 26 and 28) and just starting out (page 30). We also look back at a noteworthy chapter in our history—in this case the work of ORNL biologists Liane and William Russell, who created the first radiation exposure guidance for pregnant women or those likely to conceive (page 32).

This will be my final issue of *ORNL Review*. After exactly 10 years as ORNL's director, I am taking on a new role as senior vice president for laboratory operations at Battelle, which operates ORNL in partnership with the University of Tennessee. It has been an honor to serve with the talented staff at ORNL and to have shared in celebrating many successes over the past decade.

I look forward to many more accomplishments from this important institution in the years to come.

Thomas Mason

Thomas Mason Laboratory Director

Award-winning research owes a debt to ORNL's 'Mouse House'

ORNL's historic mouse colony had a prominent role in groundbreaking autoimmune disease research recently recognized by the Royal Swedish Academy of Sciences.

The research brought this year's prestigious Crafoord Prize in Polyarthritis to scientists in Japan and the United States "for their discoveries relating to regulatory T-cells, which counteract harmful immune reactions in arthritis and other autoimmune diseases."

David Galas, who collaborated with U.S. winner Fred Ramsdell, says ORNL's mammalian genetics program provided the "crucial piece of evidence" for identifying a gene critical to regulating immune responses.

In a letter applauding Ramsdell's win, Galas also praised ORNL's William and Liane Russell for identifying the importance of and maintaining the spontaneous mutant strain—called "scurfy"—for decades.

"With remarkable patience and foresight, they bred this strain for over 40 years. It is still unclear to me how they had the intuition to know that this was an important biological effect and therefore could lead to an important gene," Galas wrote.

Gala's letter made its way to Liane Russell, now retired and living in Oak Ridge, and the researchers renewed their correspondence.

As Galas noted, the mutation was identified in the early years of the ORNL mutant mouse colony—popularly known as the "Mouse House"—which operated from the late 1940s through 2009. In the more recent research, Galas, Ramsdell and their colleagues marshalled an effort that led to the mapping, cloning and identification of a gene recognized as of critical importance in the future of immunology.

Using the ORNL mutant strain, the research group identified the mutated gene in the scurfy mouse—the FOXP-3 gene—that controls the key genes of regu-



ORNL's Liane Russell played a key role in research that led to this year's prestigious Crafoord Prize. Image credit: ORNL

latory T-cells and thereby regulates the body's immune responses.

The Mouse House was initially established in the late 1940s to study the genetic effects of radiation exposure. The Russells were both National Academy of Science members and recipients of the Enrico Fermi Award for their groundbreaking mammalian genetics research, which included the development of occupational radiation dose limits (see "Liane Russell, pioneer of fetal rad safety," page 32)—Bill Cabage

For more information: https://go.usa.gov/xXcgf

Giant poplar dataset promising for biofuels

ORNL researchers have released the largest-ever single nucleotide polymorphism dataset of genetic variations in poplar trees, information useful to plant scientists as well as researchers in the fields of biofuels, materials science and secondary plant metabolism.

For nearly 10 years researchers with DOE's ORNL-led BioEnergy Science Center have studied the genome of *Populus*—a fast-growing perennial tree recognized for its economic potential in biofuels production.

They released the Genome-Wide Association Study dataset earlier this year. The dataset comprises more than 28 million single nucleotide polymorphisms, or SNPs, derived from approximately 900 resequenced poplar genotypes. Each SNP represents a variation in a single DNA nucleotide, or building block, and can act as a biological marker, helping scientists locate genes associated with certain characteristics, conditions, or diseases.

The data "gives us unprecedented statistical power to link DNA changes to phenotypes [physical traits]," said ORNL plant geneticist Gerald Tuskan, who presented the data at the Plant & Animal Genome Conference in San Diego. The results of this analysis have been used to



Scientists gleaned data from Populus trees in an ORNL greenhouse as part of the largest-ever single nucleotide polymorphism dataset of the species' genetic variations. Image credit: ORNL

seek genetic control of cell-wall recalcitrance—a natural characteristic of plant cell walls that prevents the release of sugars under microbial conversion and inhibits biofuels production.

BESC scientists are also using the dataset to identify the molecular mechanisms controlling deposition of lignin in plant structures. Lignin, the polymer that strengthens plant cell walls, acts as a barrier to accessing cellulose and thereby prevents cellulose breakdown into simple sugars for fermentation.—Stephanie Seay

For more information: https:// go.usa.gov/xX5CB

ORNL breaks data transfer efficiency record

ORNL researchers have set a new record in the transfer of information via superdense coding, a process by which the properties of particles like photons, protons and electrons are used to store as much information as possible.

The ORNL team transferred 1.67 bits per qubit, or quantum bit, over a fiberoptic cable, edging out the previous record of 1.63.

The work by ORNL's Brian Williams, Ronald Sadlier and Travis Humble is published as "Superdense coding over optical fiber links with complete Bell-state measurements" in Physical Review Letters. The research was selected as an "Editor's Suggestion," a distinction reserved for approximately one in six PRL papers.

Whereas computers transmit information in the form of bits (generally represented by either a 1 or a 0), qubits can employ two states simultaneously and therefore represent more information than a traditional bit. The physics of this quantum communication task employed by Williams and his team is similar to that used by quantum computers, which use qubits to arrive at solutions to extremely complex problems faster than their bitladen counterparts.

Williams' team was the first to use superdense coding over optical fiber, a major achievement in the quest to adopt

quantum communication in modern networking technology. And because the team used conventional laboratory equipment such as common fiber-optic cable and standard photon detectors, they have brought the technique one step closer to practical use.—Scott Jones

For more information: https:// go.usa.gov/xX5aH

Two elected fellows of American Nuclear Society

ORNL researchers Alan S. Icenhour and Jess C. Gehin have been elected fellows of the American Nuclear Society.

associate lcenhour. laboratory director for ORNL's Nuclear Science and Engineering Directorate, was cited for his professional leadership, which has "shaped the national R&D agenda for advanced reactor technology, nuclear fuel cycle and nonproliferation, which has led to the establishment of new isotope production and nuclear security capabilities."

Icenhour has more than 30 years' research experience in nuclear fuel enrichment, stable and radioisotope production. radioactive waste management and global nuclear security. Before joining ORNL in 1990 he served in the U.S. Navy as a commissioned officer aboard a nuclearpowered submarine and remained in the service as an active reservist until 2010. when he retired with the rank of captain.

Gehin, director of the Consortium for Advanced Simulation of Light Water Reactors, was honored for "outstanding and effective technical leadership in crossdisciplinary teams providing next-generation analyses capabilities for nuclear reactors and influencing decisions for advanced reactors and nuclear fuel cycle research and development."

Gehin came to ORNL from the Massachusetts Institute of Technology in 1992 and has been instrumental in projects such as the Advanced Neutron Source Research Reactor, Fissile Material Disposition Program, and DOE Fuel Cycle Technologies and Advanced Reactor Programs in addition to his current role with CASL, a DOE Energy Innovation Hub.





Alan S. Icenhour

Jess C. Gehin

As director of CASL, Gehin leads advanced modeling and simulation development focused on bridging the gap between basic research, engineering development and commercialization for nuclear energy reactors and fuel technology.—Sean Simoneau

Computation identifies nickel-78 as 'doubly magic'

For many of us "doubly magic" may evoke images of Penn & Teller. However, for nuclear physicists, it describes atomic nuclei that have greater stability than their neighbors thanks to having shells that are fully occupied by both protons and neutrons.

Theoretical physicists at ORNL have used Titan, America's most powerful supercomputer, to compute the nuclear structure of nickel-78, consisting of 28 protons and 50 neutrons, and found that this neutron-rich nucleus is indeed doubly magic. The results, published in Physical Review Letters, may improve understanding of the origin, organization and interactions of stable matter.

first-principle tions run on Titan, we confirmed that a very exotic nucleus about which little is known, nickel-78, is doubly magic," said theoretical physicist Gaute Hagen, who performed the study with Gustav Jansen and Thomas Papenbrock.

The term doubly magic is thought to have been coined by Eugene Wigner, former research and development director of the Manhattan Project-era facility that became ORNL. At magic numbers, which include 2, 8, 20, 28, 50, 82 and 126, either

the protons or the neutrons fill complete shells of an atom's nucleus. The shells for protons and those for neutrons are independent of each other. If the number of protons and the number of neutrons are both magic, the nucleus is said to be doubly magic.

"The binding energy, or energy needed to remove either a proton or a neutron, is larger for doubly magic nuclei compared to their neighbors," Hagen explained. The nuclear chart shows that several doubly magic isotopes—atomic elements that chemically behave identically but physically differ in numbers of neutrons—exist near the "valley of stability," the region that comprises all stable and long-lived nuclei. Examples are helium-4, oxygen-16, calcium-40, calcium-48 and lead-208.—Dawn Levy

For more information: https://go.usa.gov/xX5rd

ORNL has announed the latest for scientific computing middleware

ORNL has announced the latest release of its Adaptable I/O System, a middle-ware that speeds up scientific simulations on parallel computing resources such as the laboratory's Titan supercomputer by making input/output operations more efficient.

While ADIOS has long been used by researchers to streamline file reading and writing in their applications, the production of data in scientific computing is growing faster than I/O can handle. Reducing data on the fly is critical to keeping I/O up to speed with today's largest scientific simulations and realizing the full potential of resources such as Titan to make real-world scientific breakthroughs. And it's also a key feature in the latest ADIOS release.

"As we approach the exascale, there are many challenges for ADIOS and I/O in general," said Scott Klasky, scientific data group leader in ORNL's Computer Science and Mathematics Division. "We must reduce the amount of data being processed and program for new architectures. We also must make our I/O frame-

works interoperable with one another, and version 1.11 is the first step in that direction."—Scott Jones

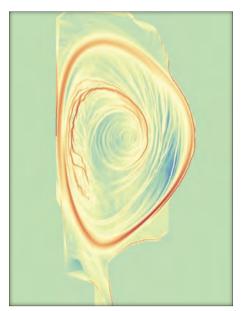
For more information: https://go.usa.gov/xX5rw

Titan supercomputer simulates nanoparticles

With the potential to increase data capacity and density, magnetic nanoparticles are promising materials for next-generation recording and storage devices like hard drives. But to make the most of new devices, scientists must understand how magnetism works at the atomic level.

Using new data from researchers at UCLA and Lawrence Berkeley National Laboratory who traced the positions of 23,000 atoms in an iron-platinum nanoparticle, ORNL computational scientists Markus Eisenbach and Paul Kent used ORNL's Titan supercomputer to simulate magnetism atom by atom from a region of the nanoparticle. The study, published in *Nature*, is the first to model the magnetic properties of a nanoparticle using real experimental data.

"These types of calculations have been done for ideal particles with ideal crystal



The bulk velocity field in a fusion simulation was computed and visualized using ADIOS. Image credit: James Kress and David Pugmire, ORNL

structures but not for real particles," Eisenbach said.

Eisenbach and Kent simulated a supercell of about 1,300 atoms from strongly magnetic regions of the nanoparticle using the award-winning LSMS code—a first-principles density functional theory code developed at ORNL.

The unprecedented simulations revealed that the energy associated with magnetic anisotropy—or the direction magnetism favors from atom to atom—transitions suddenly at boundaries created by different configurations of iron and platinum particles, an important result for focusing future studies.

Although first-principles calculations are currently too intensive to solve small-scale magnetism for regions larger than a few thousand atoms, researchers hope that computing advances will make a full-particle simulation possible in the future. More computationally intensive simulations could also show how different fabrication processes, such as the temperature at which nanoparticles are formed, influence magnetism and performance.— *Katie Elyce Jones*

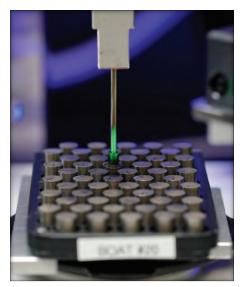
For more information: https://go.usa.gov/xXU8J

Automated measurements enhance Pu-238 production

A new automated measurement system developed at ORNL will ensure quality production of plutonium-238 while reducing handling by workers.

NASA has funded ORNL and other national laboratories to develop a process that will restore U.S. production capability of Pu-238 for the first time since the late 1980s, when the Savannah River Plant ceased production. ORNL has produced and separated about 100 grams of the material and plans to scale up the process over the next several years to meet the demand to power NASA deep space missions.

"We are bringing together multiple disciplines across ORNL to achieve this automation and ramp up so that we can



Researchers test the robotic retrieval of a raw material pellet for production of plutonium-238. Image credit: Jason Richards, ORNL

supply Pu-238 for NASA," said Bob Wham, who leads the project for the lab's Nuclear Security and Isotope Technology Division.

The Pu-238 is produced from neptunium-237 feedstock provided by Idaho National Laboratory. Workers at ORNL mix neptunium oxide with aluminum and press the mixture into high-density pellets.

automated The new measurement system robotically removes the Np-237 pellets from their holding tray and measures their weight, diameter, and height. "We're excited to go from making these measurements by hand to just pressing a 'GO' button," said Jim Miller, a scientist in the Fusion and Materials for Nuclear Systems Division who is employing the new system. "About 52 Np-237 pellets can be measured per hour using the new automated measurement system," he added.

Pellets meeting specifications. as determined by the new automated measurement system, are placed in a cassette that moves to another location for loading into a hollow aluminum tube that is hydrostatically compressed around the pellets.

The Np-237 pellets loaded in the hollow aluminum tube later enter ORNL's High Flux Isotope Reactor, where they are irradiated, creating Np-238, which guickly decays and becomes Pu-238.

The irradiated pellets are then dissolved, and ORNL staff use a chemical process to separate the plutonium from any remaining neptunium. Purified plutonium is converted back to an oxide powder, packaged and shipped to Los Alamos for final processing.

Plans are to initially produce 400 grams of Pu-238 per year on average at ORNL and then to increase that quantity through additional automation and scale-up processes.—Stephanie Seay

For more information: https:// qo.usa.gov/xXGUK

Using diamonds for drug delivery

For drugs to be effective, they have to be delivered safely and intact to affected areas of the body. Drug delivery, much like drug design, is an immensely complex task.

Cutting-edge research and development like that conducted at the ORNL can help solve some of the challenges associated with drug delivery.

ORNL researchers and collaborators at Wayne State University recently used a unique combination of experimentation and simulation to shed light on the design principles for improved delivery of RNA drugs, promising candidates in the treatment of a number of medical conditions including cancers and genetic disorders.

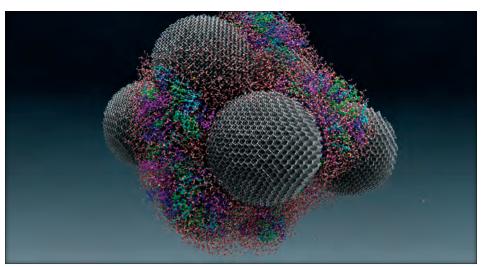
Specifically, the research team discovered that the motions of a tRNA (or transfer RNA) model system can be enhanced when coupled with nanodiamonds, or diamond nanoparticles approximately 5 to 10 nanometers in size.

Nanodiamonds are good delivery candidates due to their spherical shape, biocompatibility and low toxicity. And because their surfaces can be easily tailored to facilitate the attachment of various medicinal molecules, nanodiamonds have tremendous potential for the delivery of a vast range of therapies.

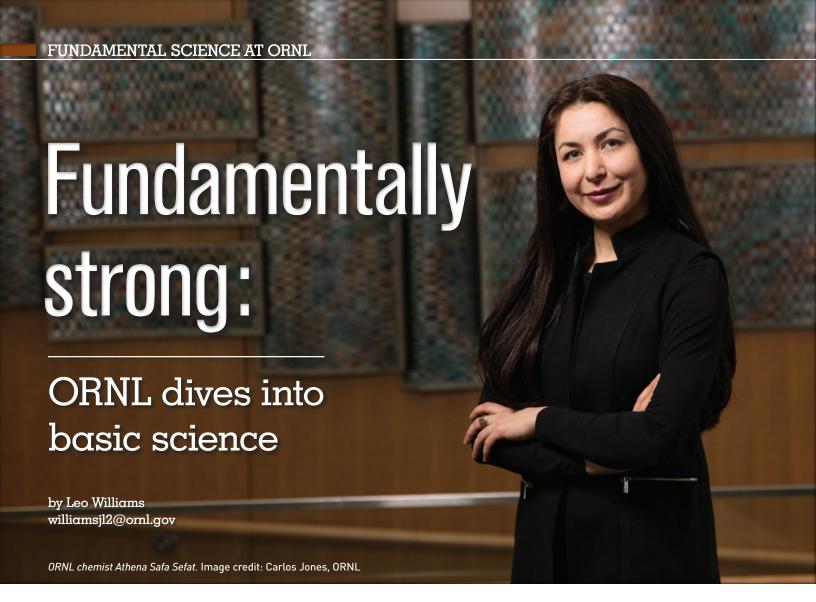
The discovery involved ORNL's Spallation Neutron Source, which provides the most intense pulsed neutron beams in the world for scientific research and industrial development, and ORNL's Titan supercomputer, the nation's most powerful for open science—a one-two punch for illuminating the physical properties of potential drugs that inform new design principles for safer, improved delivery platforms.

By comparing the SNS neutron scattering data with the data from the team's molecular dynamics simulations on Titan, the researchers have confirmed that nanodiamonds enhance the dynamics of tRNA when in the presence of water. This cross-disciplinary research was profiled in the Journal of Physical Chemistry B.—Scott Jones

For more information: https:// qo.usa.gov/xXGm6



Water is seen as small red and white molecules on large nanodiamond spheres. The colored transfer RNA can be seen on the nanodiamond surface. Image credit: Michael Mattheson, ORNL



The Dutch physicist Heike Kamerlingh Onnes discovered more than a century ago that elemental mercury can transmit electricity without energy loss, making it the first known superconductor.

The catch was that it had to be very cold—near absolute zero—and while scientists have since discovered or created higher-temperature superconductors, they have a long way yet to go. Even now, the highest-temperature superconducting wire must be cooled well below minus 200 degrees Fahrenheit to do its thing, so its use is not widespread.

Better superconductors could revolutionize how we store and distribute electric power, but we have only a tenuous understanding of what makes superconductors behave the way they do.

Superconductors fall into the category of quantum materials. Whether it's a high-temperature superconductor or a simple magnet, a quantum material behaves as it does because of what's going on at the level of atoms and their electrons. In addition, it displays its special behavior only below a specific temperature.

Why do quantum behaviors appear only below certain temperatures, and how can these transition temperatures be controlled? These are the questions at hand.

Investigating quantum behavior

"Nearly every quantum material was found serendipitously," explained ORNL chemist Athena Safa Sefat. "At room temperature they mostly don't do anything interesting.

"What are the collective chemical, electronic, and spin phenomena at atomic scales that cause superconductivity below a particular temperature in these materials? That's what we're trying to understand."

Sefat and her colleagues at ORNL bolster their experimental results on materials with theoretical modeling. And while superconductors hold enormous promise—because of their ability to transmit very large amounts of electricity without loss, creating exceptionally strong magnetic fields—the team's efforts go beyond the practical to a fundamental exploration of the nature of quantum materials and the functionality of matter.

"This is what fundamental science is trying to understand," she said. "What is it about the local chemical, electronic, and spin structures—as well as other factors—that combine to make a material superconducting below a critical temperature in a bulk sample?"

See FUNDAMENTALLY STRONG, page 8

Oak Ridge Leadership Computing Facility

Tackling big questions with computation

by Sean Simoneau ornlreview@ornl.gov

or some researchers, cracking the big questions can be like mining for a lone diamond under tons of solid rock.

In those situations it helps to have a good set of tools, particularly the Oak Ridge Leadership Computing Facility and its Titan supercomputer.

Titan isn't the facility's first world-class computing system. The OLCF was established in 2004 to develop a supercomputer more advanced and powerful than any machine at the time, and it has since hosted several that were among the world's most powerful. In addition, staff at the facility provide a suite of data analysis and visualization tools to meet diverse scientific needs.

The OLCF's current system is Titan, a 27-petaflop Cray supercomputer capable of performing 27,000 trillion calculations per second, making it the most powerful supercomputer in the U.S. and the No. 3 computer in the world, behind two in China. Titan boasts a unique hybrid architecture that combines traditional central processing units with graphics processing units; GPUs were first developed to speed computer video but have also proven lightning fast in scientific computing.

OLCF users come from a variety of institutions worldwide, including universities, private industry and other government labs. They also bring a wide variety of scientific problems, from traditional explorations in physics, materials science and chemistry, to fusion energy, plasma engineering and climate modeling.

In recent years the OLCF has seen strong growth in emergent areas such as systems biology and data-intensive science. In addition, the facility has seen an increase in experimental analysis from researchers at other DOE user facilities.

"We're as broad as science is broad," said Jack Wells, science director at ORNL's National Center for Computational Sciences, which houses the OLCF. "We want a vibrant user community. We don't want it to get stale."

OLCF's unparalleled capabilities are in high demand; the facility receives almost three times as many proposals as it can accommodate.

In 2018 OLCF will deliver the Summit supercomputer, providing more than five times the computational power of Titan along with greater speed and efficiency. The OLCF is also working on DOE's Exascale Computing Project to prepare for the world's first high-performance computing system capable of at least a billion billion calculations per second.

"OLCF is unique because we are very productive and we have delivered our resources on time, on scope and on budget," Wells said. "In the future we will develop greater complexity to produce more valuable and more meaningful results for bigger, more complicated hierarchical questions."



Titan supercomputer. Image credit: Andy Sproles, ORNL

FUNDAMENTALLY STRONG, from page 6

A collaborative lab

The work of Sefat and her colleagues belongs to a long tradition of fundamental research at ORNL. Born of the government's drive during World War II to create nuclear weapons, ORNL has grown to become the DOE Office of Science's largest and most diverse laboratory.

Indeed, of 24 core capabilities recognized by the Office of Science—skills such as applied mathematics and advanced instrumentation as well as many areas of physics, chemistry, biology, engineering, earth sciences and computing—ORNL lays claim to 23, the most of any DOE science lab. Thomas Zacharia, the lab's deputy for science and technology, ORNL's diversity makes it uniquely able to tackle science's most difficult challenges.



Thomas Zacharia

"I think the laboratory is fundamentally distinguished by team science," he said, "asking more of the bigger questions that require a team of people from different fields of science, different expertise, different capabilities."

This diversity can be seen in the range of accomplishments coming from ORNL researchers. A team of scientists from the Chemical Sciences Division and the lab's Spallation Neutron "That is truly fundamental science," Zacharia said. "It's not every day that you change the periodic table, and the work that was done here is going to change the periodic table in every text-book in the world."

Unprecedented scientific tools

ORNL's collaborative environment is distinguished not only by the talent and diversity of its staff but also by the tools at their disposal, unique facilities that allow researchers to interrogate matter at a level that would otherwise be impossible.

ORNL hosts a number of DOE Office of Science user facilities. These include two leading neutron science facilities, the Spallation Neutron Source and the High Flux Isotope Reactor (which was instrumental in the discovery of tennessine); the Center for Nanophase Materials Sciences, which supports nanoscience with broad capabilities in synthesis, characterization, microscopy and theory; and the Oak Ridge Leadership Computing Facility, which is home to the country's most powerful supercomputer, Titan.

"These are unique, world-leading scientific facilities," Zacharia said. "They require not only a team of scientists to operate but also a team approach to tackle the fundamental questions that require these types of facilities, because each of these facilities allows us to probe matter or ask questions at a deeper level."

The lab's collaborative approach—and its advanced tools—can be seen in the work of Sefat and her collaborators in exploring superconductivity.

Sefat herself, a solid-state chemist working in a materials group, uses insights from her team to create custom crystals in atomic configurations that may be promising. While they don't know for certain how superconductivity comes about, they do have clues; for instance, high-temperature superconductors all start with antiferromagnets (materials whose atoms have magnetic

"These are unique, world-leading scientific facilities. They require not only a team of scientists to operate but also a team approach to tackle the fundamental questions that require these types of facilities, because each of these facilities allows us to probe matter or ask questions at a deeper level."

ORNL Deputy for Science and Technology Thomas Zacharia

Source recently announced they had discovered a new state of water molecules—neither solid, liquid nor gas—under extreme confinement (see go.usa.gov/x9GEH). Elsewhere at the lab researchers are using their expertise in computational science to promote cancer research by mining data from cancer reports to reveal promising approaches that might have been overlooked (see go.usa.gov/x9Gm2).

Perhaps most visibly, ORNL was a key player in the collaboration that discovered tennessine, an element with atomic number 117 (see go.usa.gov/x9GmG).

directions opposite those of their neighbors), are similarly layered, and have a small amount of chemical doping that creates some level of disorder.

Because of her expertise Sefat is able to take a material and replace atoms at specific sites throughout its structure. Then she does the first tests of a material herself, measuring bulk properties such as its resistance, its response to a magnetic field, changes in its crystal structure, and its transition temperature.

Colleagues at ORNL's Center for Nanophase Materials Sciences get a nanoscale look at the material's electronic struc-

See FUNDAMENTALLY STRONG, page 10



levyd@oml.gov

Researchers sometimes need access to expertise and facilities not available at their universities, companies and institutes. To manipulate materials on the scale of nanometers—billionths of a meter—they come to the world-class experts, specialty instruments and state-of-the-art techniques at ORNL's Center for Nanophase Materials Sciences.

Each year about 600 researchers worldwide come to CNMS to advance their work. A peer-reviewed proposal secures access to capabilities from materials synthesis and assembly, to imaging and characterization, to theory, modeling and simulation. CNMS staff support visiting scientists throughout their research.

"Most users are surprised by just how much can be done here," CNMS Director Hans Christen said. His team focuses on helping users succeed, but ORNL staff also conduct their own research on materials that capture, transport and convert energy.

CNMS began operations in 2006. Because it is near ORNL's neutron science and high-performance computing facilities, users can integrate these unique tools into their experiments. In fact, one-sixth of CNMS users also make use of ORNL's neutron facilities.

The center's nanofabrication research laboratory features clean rooms with tools for building structures at the nanoscale to

microscale (billionths to millions of a meter). "We're approaching the ability to control structure precisely over nanometers to meters," CNMS's Michael Simpson said. "With cutting-edge technologies we're developing, we are pushing down to the molecular scale. The ultimate goal is to be able to define the position of every atom within very complex systems."

"We're approaching the ability to control structure precisely over nanometers to meters."

- CNMS materials scientist Michael Simpson

Advanced instruments—for microscopy, spectroscopy, tomography and more—let users investigate and understand nanomaterials at a whole new level.

"When users come to the CNMS, they have access to all of these techniques and the experts who invented them," said Stephen Jesse, who develops techniques for scanning probe microscopes.

Liz Norred from the University of Tennessee used CNMS to fabricate microfluidic devices for rigorous analysis of gene expression. "It's rare to see so many resources all in the same facility," she said. "It's even rarer to have so many people willing to help you with those resources."

For more information: https://www.ornl.gov/facility/cnms

FUNDAMENTALLY STRONG, from page 8

ture through scanning tunneling spectroscopy. Materials also are subjected to neutron analyses at the lab's two neutron facilities, which provide information on spin structures, ordering types and magnetic excitations.

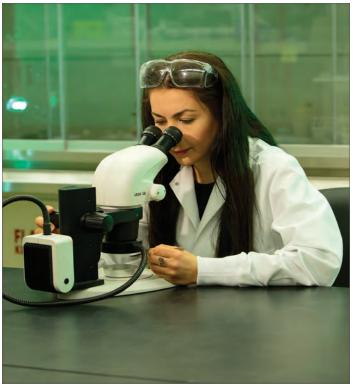
Meanwhile these experimental results are supported by models done by theoreticians at the lab.

"This is fundamental science, where we aim to understand the causes of a material's quantum behavior by probing it near its transition temperature."

- ORNL chemist Athena Safa Sefat

"Once you synthesize the crystal, you can study properties and see whether your hypotheses have worked or not," Sefat explained. "That's a loop that goes around: What did I change? What property has it manifested? Then you go back, make a change, and take another look at the properties and theoretical explanations."

Ultimately the team's work is likely to help make a class of very valuable materials—superconductors—even more so, but it will also help us answer essential questions. For instance, how and why does temperature play such a crucial role in the way matter behaves?



Athena Safa Sefat. Image credit: Carlos Jones, ORNL

potentially design improved materials to function specifically at desired temperatures."

Of course the nature of superconductors and other quantum materials is only one of the mysteries waiting to be revealed,

"I see this laboratory emerging as a vanguard of scientific institutions, not only in this country but globally. My vision for this laboratory is that it be the place where the best minds will want to come to be part of this enterprise."

— ORNL Deputy for Science and Technology **Thomas Zacharia**

"This is fundamental science, where we aim to understand the causes of a material's quantum behavior by probing it near its transition temperature, Sefat said."

The importance of temperature is important in our everyday lives as well, she noted.

"As you warm things up, some transform into a liquid while others stay solid, so temperature really matters—as well as other parameters such as applied magnetic field and pressure. In my research we're really trying to understand what's determining the transition point between what it is and what it becomes. Understanding such causes through fundamental science, we can

and ORNL researchers will be deeply involved in many of these explorations. $\,$

"I think this laboratory is poised to do even more remarkable things," Zacharia said, pointing to efforts such as the development of exascale supercomputers that perform more than a billion billion calculations each second, or quantum computers that use the behavior of individual atoms to solve especially difficult problems, or new technologies for providing nuclear energy.

"I see this laboratory emerging as a vanguard of scientific institutions, not only in this country but globally," Zacharia said. "My vision for this laboratory is that it be the place where the best minds will want to come to be part of this enterprise."

ORNL's Neutron Science User Facilities

Neutrons unlock the mysteries of materials

by Sean Simoneau ornlreview@ornl.gov

n 1944 ORNL physicist Ernest Wollan proposed a novel lacksquare method for using neutrons to study the atomic structure of materials. At the Graphite Reactor—then known as the X-10 Pile—Wollan worked with future Nobelist Clifford Shull to pioneer neutron-scattering research and unlock the potential of neutron diffraction.

Today ORNL is home to the most advanced neutron research facilities in the world. The accelerator-based Spallation Neutron Source provides the world's most intense pulsed neutron beam, producing brighter neutrons for sensitive, detailed experiments, while the High Flux Isotope Reactor has the country's highest steady-state thermal and cold neutron fluxes for neutron diffraction, isotope production and material irradiation studies.

Together they combine cutting-edge instrumentation with powerful data analysis and visualization software, helping researchers from across the globe better understand the structure and property of materials.

"The primary mission of SNS and HFIR is to provide open access to sophisticated instrumentation needed to probe and create materials for scientists of many disciplines," said Alan Tennant, chief scientist for ORNL's Neutron Sciences Directorate and director of the Shull Wollan Center, a Joint Institute for Neutron Sciences.

ORNL's neutron facilities are known for their unique and superlative capabilities. The two facilities have a total of 30 instruments, each uniquely designed for specific types of experiments, samples and environments.

Neutron diffraction is a crucial tool in both the physical and life sciences, used to study everything from battery components to cellular structures to additively manufactured (3-D-printed) materials.

ORNL's neutron facilities serve thousands of users and visiting researchers every year from academia, national laboratories and industry. The selection process is competitive only one in three proposals is awarded time—but the data gained from SNS and HFIR experiments can offer insight not available using other techniques.

"Our neutron facilities provide unique capabilities to the scientific community critical to maintaining ORNL leadership in the physical sciences," Tennant said.

The next big step for ORNL's neutron user facilities is a proton power upgrade at SNS that will increase neutron flux at the current target station and provide a necessary platform for construction of a Second Target Station. The STS will complement and boost the lab's existing abilities with a new suite of tools, such as intense cold neutrons, that will keep the U.S. competitive with new neutron facilities in Europe and Asia.



Neutrons and quantum spin liquids: Exploring the next materials revolution

by Jeremy Rumsey rumseyjp@ornl.gov

Neutrons have for decades helped us understand the exotic electronic and magnetic properties of quantum materials such as high-temperature superconductors and other materials that behave beyond the boundaries of classical physics.

"A revolution in quantum materials is happening now," said Alan Tennant, chief scientist for ORNL's Neutron Sciences Directorate. "We're looking at their properties with a new set of concepts that promise new technologies in the future, and neutrons play a central role in this."

The study of quantum materials spans a wide range of physics domains and applications. ORNL's neutron facilities—the High Flux Isotope Reactor and Spallation Neutron Source—are proving especially useful, allowing condensed matter physicists to make remarkable discoveries related to a novel state of matter called quantum spin liquid.

QSLs consist of groups of correlated electrons that behave like tiny microscopic magnets that physicists call "spins." The electrons in traditional magnets spin in a parallel arrangement throughout the material, forming a cohesive magnetic moment. However, the "frustrated" spins in QSLs demonstrate a liquid-like behavior and do not align in an orderly fashion as you would expect in a solid material—kind

of like if water refused to freeze even in freezing temperatures.

"Where we've really contributed something new at the forefront is in finding excitations associated with a special type, called Kitaev QSLs," said Steve Nagler, director of ORNL's Quantum Condensed Matter Division. "They've attracted a lot of attention in recent years because of their possible relation to quantum computing."

Researchers suspect that if the exotic behavior of the Kitaev QSL can be harnessed, it might provide a potential platform for quantum bits—or qubits—that could revolutionize computing. While traditional bits contain only single pieces of information in the 1s and 0s of a computer's binary code, qubits have no such limitation.

Nagler was part of the group that identified magnetic excitations associated with the Kitaev QSL in a two-dimensional graphene-like material in 2016, a decade after physicist Alexei Kitaev developed his theoretical model. The paper detailing their discovery was a cover story in *Nature Materials*, and *Discover Magazine* ranked it 18th on its list of the 100 most significant research stories of 2016.

Because neutrons have their own magnetic moment but carry no charge, they are ideal for characterizing magnetic behavior in almost any material without compromising the material's integrity.

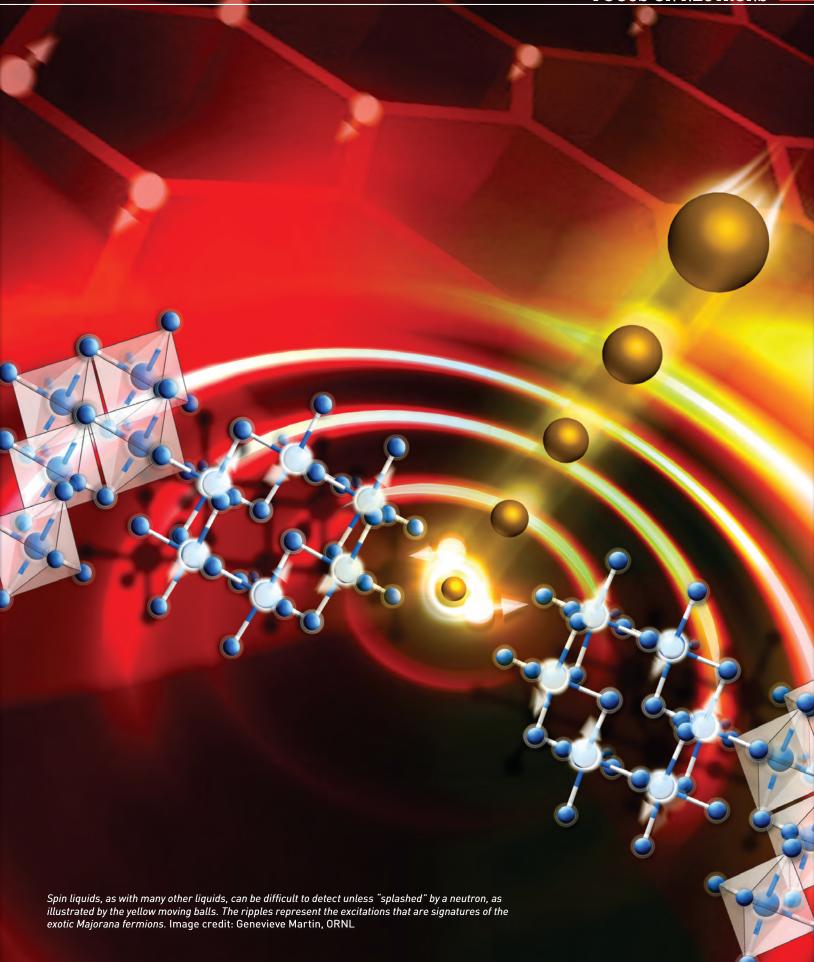
"Neutrons are especially adept at characterizing how spins interact with each other through space and time, which are exactly the two things you need to measure magnetic excitations such as those in the Kitaev QSL," Nagler said. "Our state-of-the-art neutron scattering capabilities, combined with our rich user program, have really allowed us to make some impressive additions to the knowledge of these things."

Researchers around the world are using ORNL's suite of neutron scattering instruments to reveal fundamental details such as

- the key ingredients underpinning QSLs' exotic magnetic behavior;
- new insights into spinons—entities that carry electron spin information; and
- new characterizations of quantum phase transitions, explaining how quantum behavior affects changing states of matter.

ORNL's Shull Wollan Center is helping to prime discovery by pairing experimentalists with theorists working on the latest developments. It's a partnership that Tennant, the center's director, says is necessary to a field that is moving so quickly.

"If silicon and superconductors were the start of a second quantum revolution where quantum effects beyond single atoms were harnessed," Tennant said, "then what we're looking at here is a kind of third quantum revolution, where we control and manipulate highly entangled quantum states. This promises to deliver new technologies that are going to define the next 50 to 100 years."



Lab in a gold mine

looks at matter-antimatter imbalance

by Leo Williams williamsjl2@ornl.gov

There's a problem with our understanding of the universe: We don't know why it has enough matter to make it interesting.

The Standard Model of particle physics encompasses three of nature's four fundamental forces—all but gravity—yet it tells us the Big Bang should have produced matter and antimatter in equal measure. Therefore, the two should have cancelled each other out, leaving a universe with energy but essentially no matter: no galaxies, no planets, no us.

Clearly the Standard Model is missing something; figuring out what that might be is one of the great challenges of modern science.

"The fact that we're here talking about it means that that didn't happen," noted ORNL physicist David Radford, "So there must have been some imbalance bigger than what was predicted by the equations—quite a bit bigger."

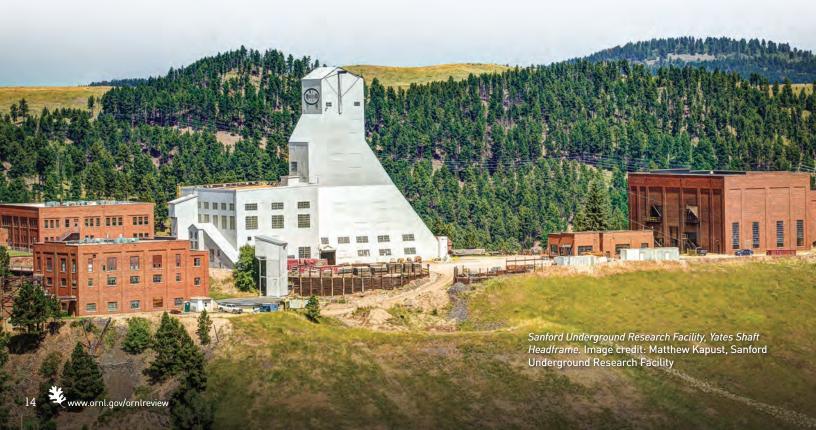
A team co-led by Radford created a lab 4,850 feet underground at South Dakota's Sanford Underground Research Facility to help them find the glitch. There, in a retired gold mine, they will focus on nature's smallest known particles: neutrinos.

Neutrinos are so unassuming that trillions produced by the sun go through your

body every second without notice. They may explain the universe's matter-antimatter imbalance because they may be their own antiparticles, a theory put forward by Italian physicist Ettore Majorana 80 years ago. If he was right, neutrinos could have tipped the balance of matter over antimatter after the Big Bang.

Radford's team is working to verify Majorana's theory by establishing the conditions necessary to confirm a theoretical nuclear reaction called neutrinoless double beta decay.

When an atom goes through regular double beta decay, two neutrons in its nucleus spontaneously transform into protons, accompanied by the emission of two electrons and two neutrinos. Majora-



na's theory, however, says that if neutrinos are their own antiparticles, then double beta decay would sometimes happen without the emission of neutrinos. If we can prove the existence of neutrinoless double beta decay, we will demonstrate that neutrinos are their own antiparticles.

The team knows exactly what a neutrino-free decay would look like in its detectors. Nevertheless, such reactions, if they exist at all, are so rare that identifving them will be much more difficult than finding a needle in a haystack.

The South Dakota project—known as the Majorana Demonstrator Projecthouses 40 kilograms of detectors made from germanium, primarily the isotope germanium-76. Its primary goal is to show that other nuclear reactions—those caused by cosmic rays, for instance—can be minimized in the detectors.

This is necessary because neutrinoless double beta decays are rare. Germanium-76 has a radioactive half-life more than 100 billion times longer than the age of the universe, so even though the next experiment will contain 1 ton of germanium detectors, researchers expect to see the neutrino-free decay in only about one atom per year. Over the course of a 10-year experiment, then, they hope to see about 10 or so neutrinoless double beta decays total.

The demonstrator's detectors have been operating since October, and so far researchers are confident they will be able to sufficiently minimize background radiation.

According to DOE's Nuclear Science Advisory Committee, the experiment might answer one of the universe's most compelling mysteries.

"A ton-scale instrument designed to search for this as-yet-unseen nuclear decay will provide the most powerful test of the particle-antiparticle nature of neutrinos ever performed," the committee said in its 2015 long-range plan.

Radford agrees.

"These are perhaps the most compelling questions in all of fundamental physics right now: 'Are neutrinos their own antiparticle, and what gives rise to the excess matter in the universe?" \$







The Majorana Demonstrator is located 4,850 feet below ground in a retired gold mine (top). The demonstrator consists of an enclosure shielded by layers of rock, nitrogen, lead and copper (center) and holding detectors made of germanium-76 (bottom). Image credit: Matthew Kapust, Sanford Underground Research Facility

Why is there matter?

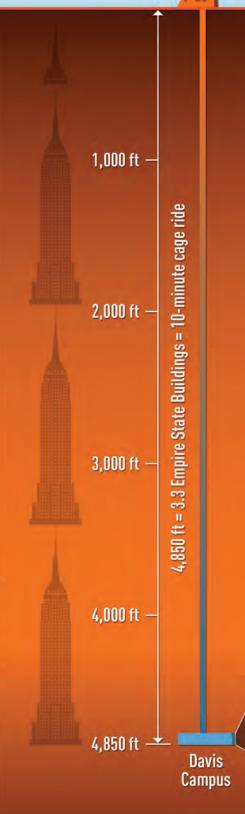
Yates headframe (houses pulley wheels, etc.)

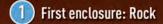
The Majorana Demonstrator is a step toward verifying that neutrinos are their own antiparticles, a discovery that might explain why matter and antimatter didn't cancel each other out in the very early universe.

The demonstrator is located 4,850 feet underground in a retired gold mine at South Dakota's Sanford Underground Research Facility. Its job is to show us how to detect a very rare type of nuclear reaction called "neutrinoless double beta decay."

How rare? The material in Majorana's detectors, germanium-76, has a radioactive half-life 100 billion-plus times the age of the universe, yet the neutrinoless events would occur even less often (if at all).

To confirm such a rare event, researchers must ensure nothing else is going on in their detectors. Here is how they use a series of concentric enclosures to shield the demonstrator from outside influence.





Nearly a mile of rock serves to block muons created by the interaction of high-energy cosmic rays with the earth's atmosphere.

Second enclosure: Polyethelene

Polyethelene shielding blocks neutrons created by reactions within the rock.

3) Third enclosure: Muon veto panels

Not a shield as such, these plastic panels warn researchers when muons created by cosmic rays make it to the experiment and allow them to disregard the resulting signal.

Fourth enclosure: Nitrogen

Radiation from the natural radon found in air is enough to interfere with the experiment. In response, pure nitrogen is pumped into a stainless steel enclosure surrounding the experiment, pushing the air (and accompanying radon) out.

Fifth enclosure: Lead

An enclosure of lead bricks blocks gamma rays emanating from the surrounding rock.

Sixth enclosure: Commercial copper

This layer of copper blocks gamma rays created within the lead bricks.

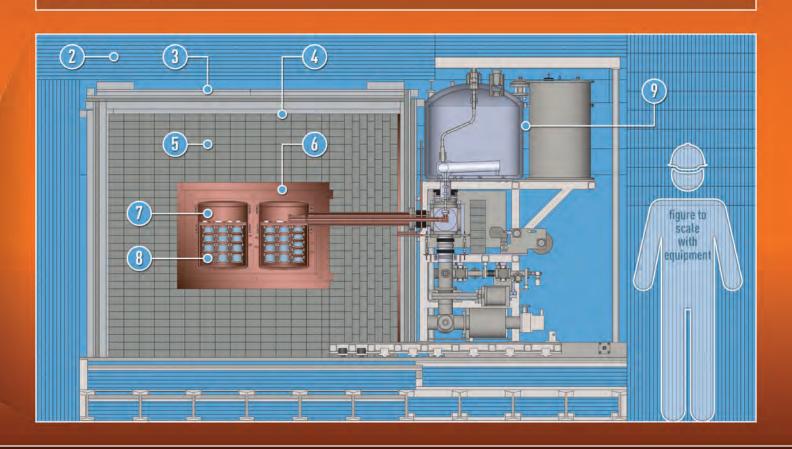
Seventh layer: Custom-purified copper

This layer blocks gamma rays from the layer of commercial copper.

The detectors

Forty kilograms of detectors made primarily from germanium-76 sit within a vacuum container cooled with liquid nitrogen to -320°F.

Cryogenics, vacuum system, electronics



Cancer research

accelerates via deep learning

by Jonathan Hines hinesjd@ornl.gov

linical trials—studies that involve human subjects—play an important role in cancer research, supplying the data necessary to evaluate, develop and improve cancer treatment. Historically, however, fewer than one in 20 cancer patients participate in clinic trials.

"Today we're making decisions about the effectiveness of treatment based on a very small percentage of cancer patients, who may not be representative of the whole patient population," said Georgia Tourassi, director of ORNL's Health Data Sciences Institute.

To expand the amount of useful data available to researchers, Tourassi and colleagues are using supercomputers to automate the information gathering needed to monitor cancer at the population level. Their project is part of the Joint

Design of Advanced Computing Solutions for Cancer collaboration between DOE and the National Cancer Institute.

Today much of the data used in cancer research must be manually curated from text-based reports by organizations that systematically collect demographic and

as deep learning could help alleviate this backlog by giving computers the ability to mimic human learning and intelligence. Using the Oak Ridge Leadership Computing Facility's Titan supercomputer, Tourassi's team applied deep learning to extract useful information from cancer

"Intuitively this makes sense because carrying out the more difficult objective is where learning the context of related tasks becomes beneficial. Humans can do this type of learning because we understand the contextual relationships between words. This is what we're trying to implement with deep learning."

— Health Data Sciences Institute Director Georgia Tourassi

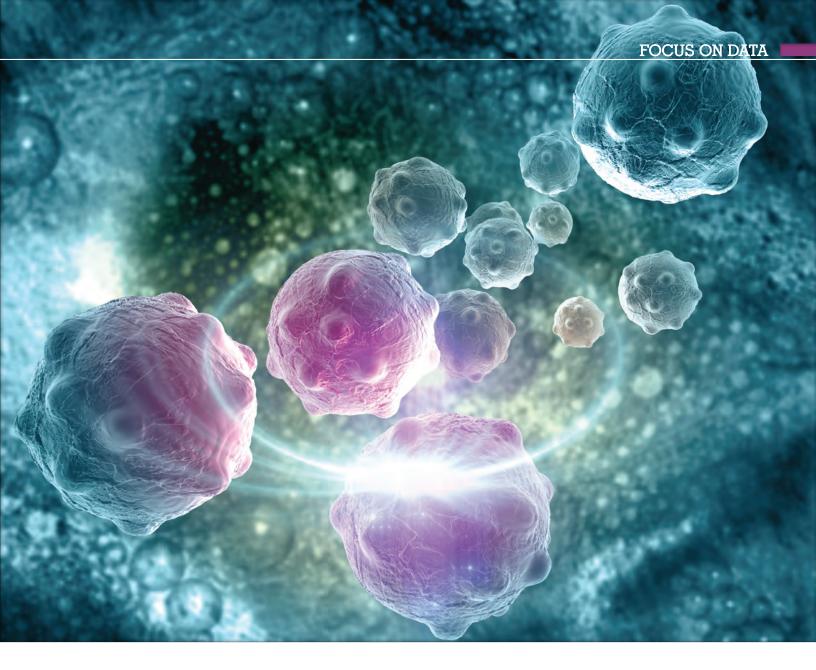
clinical information related to cancer incidence in the United States. With millions of new reports being produced each year, the information burden continues to grow.

Applying natural language processing and a machine-learning technique known

pathology reports, a foundational element of cancer surveillance.

Working with a dataset of 1,976 pathology reports provided by the cancer institute, Tourassi's team trained a deep learning algorithm to carry out two





different but closely related informationextraction tasks. In the first the algorithm scanned each report to identify the primary location of the cancer. In the second the algorithm identified the cancer site's laterality—or the side of the body on which the diseased tissue was located.

The team set up a neural network a web of weighted calculations designed to produce informed guesses on how to correctly carry out tasks—allowing it to exploit information shared by the two tasks. As a result its algorithm performed substantially better than competing methods.

"Intuitively this makes sense because carrying out the more difficult objective is where learning the context of related tasks becomes beneficial," Tourassi said. "Humans can do this type of learning

because we understand the contextual relationships between words. This is what we're trying to implement with deep learning."

Another study carried out by Tourassi's team made use of 946 cancer institute reports on breast and lung cancer to tackle an even more complex challenge: using deep learning to match the cancer's origin to a corresponding topological code, a classification that's even more specific than a cancer's primary site or laterality.

The team tackled this problem by building a convolutional neural network, a deep-learning approach traditionally used for image recognition, and feeding it language from a variety of sources. Text inputs ranged from general (e.g., Google search results) to domain-specific (e.g., medical literature) to highly specialized

(e.g., cancer pathology reports). The algorithm then took these inputs and created a mathematical model that drew connections between words, including words shared between unrelated texts.

Comparing this approach to more traditional classifiers, the team observed incremental improvement in performance as the network absorbed more cancer-specific text.

These preliminary results will help guide Tourassi's team as it scales up deeplearning algorithms to tackle larger datasets and with less supervision, meaning the algorithms will make informed decisions with less human intervention.

For more information: http:// go.usa.gov/x9mmG

Experiment re-creek the universe's first split second experiment re-creates

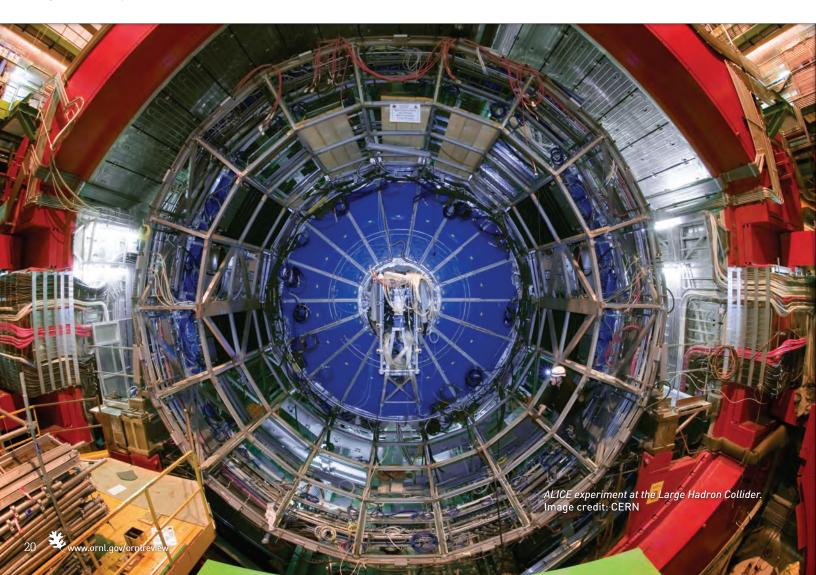
by Leo Williams williamsjl2@ornl.gov

magine back nearly 14 billion years. The universe was very small, very hot and very dense. Then it exploded in the Big Bang, quickly producing the protons and neutrons that would eventually constitute nearly all matter in the galaxies and planets we know.

For the first tiny fraction of a second, however, matter was in a form that we almost never see, a form that we didn't even postulate until the 1960s. Before about a millionth of a second after the Big Bang, the universe was a soup of tiny particles known as quarks and their force carriers, known as gluons.

Quarks and gluons are still around, but we don't observe them because they hate to be alone. By the rules of the strong nuclear force, they always combine into protons, neutrons and related particles.

"This feature of quarks and gluons, that they're particles but you can't observe them as free particles, is something that scientists have tried to understand for a long time," said ORNL physicist Tom Cormier. "It's not even fully



understood theoretically how that comes about, how something can be hidden like that and rigorously turn back into an ordinary particle before you see it."

A direct study of quarks and gluons would be very useful to anyone interested in matter and its origins, but such a study requires researchers to re-create that soup of guarks and gluons—technically known as a plasma. That is the job of the international ALICE experiment at the Large Hadron Collider, located along the border of France and Switzerland.

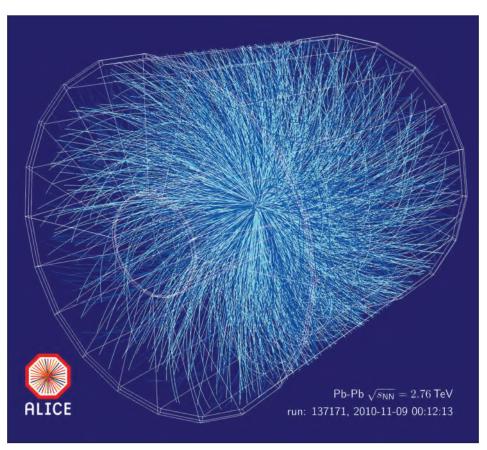
Cormier leads the American contribution to ALICE, which produces quark-gluon plasmas by accelerating lead nuclei along a 17-mile tunnel and smashing them together at essentially the speed of light. The resulting collisions create temperatures 100,000 times hotter than the core of the sun and, for a brief instant, quark-gluon plasmas.

The plasmas themselves are very, very dense, but some of the quarks and gluons-known collectively as "partons"—escape and head toward the surrounding detectors.

They don't arrive as quarks and gluons. Rather, the fastest-moving escapees create jets of more mundane particles—jets rather than single particles because they carry an enormous amount of energy. It is these secondary particles that travel through chambers filled with ionized, electrified gas, leave detectable tracks, and reach other detectors beyond.

Even though the detectors don't see quarks and gluons directly, ALICE researchers have gained an unprecedented understanding of the quarkgluon plasma through the analysis of these other particles, a process that has been likened to re-creating the workings of Swiss watches by smashing them together at the speed of light and examining the leftover pieces.

"The way those partons are scattered out into the medium, how they lose energy as they are propagated out into the medium, gives you an entirely new window on aspects of the strong interac-



Particle tracks from the collision of lead nuclei at nearly the speed of light. Image credit: CERN

tion that you have no other way to see," Cormier explained. "These hard-scattered partons turn into jets, and you're basically able to use them as a diagnostic probe of the quark-gluon plasma itself."

They are also adding to the field of computer science because of the mountain of data produced by the experiment. In fact, once ALICE is upgraded in the next several years, its detectors will

"This feature of quarks and gluons, that they're particles but you can't observe them as free particles, is something that scientists have tried to understand for a long time. It's not even fully understood theoretically how that comes about, how something can be hidden like that and rigorously turn back into an ordinary particle before you see it."

ORNL physicist Tom Cormier

For instance, researchers have discovered that the plasma behaves not like a gas—similar to an electromagnetic plasma—but like a liquid. What's more, it's a "perfect" liquid, with essentially no viscosity—less even than a superfluid such as liquid helium, which is able to climb over the sides of its container.

produce 50,000 snapshots of colliding nuclei-amounting to about a terabyte of data-each second.

"It's a real challenging problem," Cormier explained. "You can't store it all; you have to analyze it on the fly. There are a lot of computer people working on that." 🐝

Superior supercomputer parallelism for subatomic particle research

by Eric Gedenk ornlreview@ornl.gov

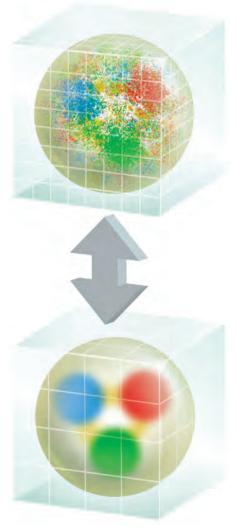
Before the 1950s, the atom's electrons, neutrons, and protons were the smallest confirmed units of matter. More recently, however, advancements in experimental and theoretical techniques allow researchers to understand even smaller particles at a more fundamental level.

The newest of these experiments lies in Hall D of the Thomas Jefferson National Accelerator Facility, also known as Jefferson Lab. There, researchers hope the GlueX experiment can offer unprecedented insight into subatomic particle interactions.

"We believe there is a theory that describes how elementary particles (known as quarks, gluons, and mesons) interact and make up the matter around us," said Robert Edwards, senior staff scientist at Jefferson Lab. "If so, the theory of quantum chromodynamics suggests that there are exotic forms of matter that exist, and that's what we're looking for in our Hall-D experiment."

Edwards and colleagues use ORNL's Titan supercomputer to inform the GlueX experiment and corroborate its findings. The team also uses Titan to improve computer codes for quantum chromodynamics, or QCD.

QCD is the study of the strong nuclear force, one of the universe's four fundamental forces (along with gravity, elec-



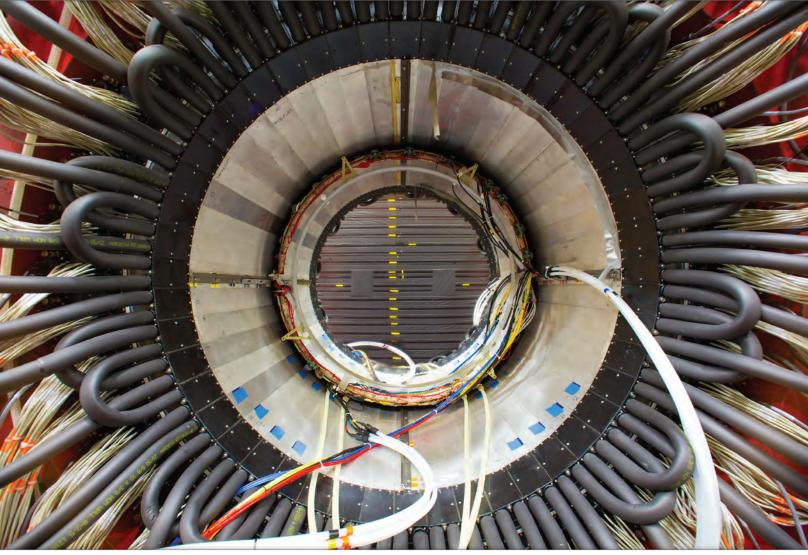
Artist's depiction of the QCD multigrid method. The top image is the fine grid, which allows the team to simulate the high-frequency noise of a proton simulation. The bottom image represents the coarse grid, which supports low-energy, long-distance modes that slow down solvers. Image credit: Jefferson Lab

tromagnetism and the weak force, which controls radioactive decay). The strong force acts between two major categories of subatomic particles—quarks and gluons. Quarks combine to form protons, neutrons and other hadrons, held together by gluons.

In addition, quarks can bind with their inverse, antiquarks, to form mesons. Mesons are among the most mysterious subatomic particles, as researchers can detect their existence for only fractions of a microsecond. Through experiments, Edwards's team hopes to use GlueX to confirm the existence of "exotic" mesons, or mesons that do not behave as QCD theory suggests they should.

Simulating the interactions of a quantum system of quarks, gluons and mesons requires a lot of computing muscle. The team has to calculate many interactions between individual particles—mapped to a grid, or lattice—then take snapshots of the model at microsecond intervals. The team takes 300–500 snapshots during a simulation.

Such computing demands push even the world's fastest supercomputers to their performance limits. The Jefferson Lab researchers have long collaborated with NVIDIA high-performance computing researcher Kate Clark to improve performance for common QCD applications. On Titan, the team focuses on increasing computer parallelism—using multiple processors to work simultaneously on different parts of a larger problem.



A view of the GlueX apparatus in Hall D, the newest experimental hall at Jefferson Lab. Scientists built GlueX to study "exotic" mesons, particles that are predicted to exist but have never before been seen. Image credit: Jefferson Lab

Similar to sound waves, which are actually composed of many individual waves that have different pitches or frequencies, the team's problem is composed of many allows them to separate the different energy states within a simulation. They can then simulate the lower-energy states on one grid and the higher-energy states

"Going forward, supercomputers like Summit will have more processing cores, so to get high efficiency, researchers in many fields are going to have to work on how to exploit all the levels of parallelism in a problem."

— High-performance computing researcher Kate Clark

configurations, or modes, with different energies. Rather than try to do all of these calculations on one grid, the researchers developed a computational workflow that

on another, allowing them to quickly get through a long line of calculations.

The team's algorithmic innovations are already paying dividends. The researchers saw up to a hundredfold speedup on their largest grids and a tenfold speedup for the finer, more detailed grids.

Edwards and his colleagues are also excited to begin working to improve parallelism on ORNL's next supercomputer, Summit, set to be delivering science in 2018.

"Going forward, supercomputers like Summit will have more processing cores, so to get high efficiency, researchers in many fields are going to have to work on how to exploit all the levels of parallelism in a problem," Clark said. \$

For more information: http:// go.usa.gov/x9mtp

Quantum materials

promise exciting technologies for energy and electronics

by Dawn Levy levyd@ornl.gov

rom the Stone, Bronze and Iron Ages to the silicon behind the Information Age, materials have defined technologies and driven economies.

Looking forward, our next epoch may lie in quantum materials.

Quantum materials respond to weak inputs with strong outputs, promising ultrathin electronics, ultrasensitive sensors and switches, smart building components and unprecedented efficiencies for technologies in energy generation, transmission and storage.

At ORNL, specialized facilities—along with expertise in materials synthesis and imaging, neutron science, theory and simulation—enable the exploration of quantum materials from graphene to quantum spin liquids.

On a fundamental level, every material is a quantum material. To describe what a magnet does, you don't need to know quantum mechanics, but to describe why a material is magnetic, you do. (Magnetism results when angular momenta of individual electrons, called "spins," align.)

That said, two aspects really set quantum materials apart from mainstream materials. "Quantum materials have properties that are strongly dependent on things that happen at very small energy scales and that are very different from what you would get if you were only to look at the average of all the electrons," said Hans Christen, director of the Center for Nanophase Materials Sciences at ORNL.

Electrons in mainstream materials are like shoppers at a mall. Individual electrons mill about the crowd predictably in classical phases of liquid, gas or solid. Electrons in quantum materials, in contrast, are like flash mobs; their actions are coordinated but defy average crowd behavior.

"For quantum materials, things that normally are not organized can become 'coherent' and move together in ways that can't be understood in terms of individuals," said James Morris, group leader in ORNL's Materials Science and Technology Division. The classic example is superconductivity, which happens only as a consequence of correlations.

In normal materials, defects scatter electrons and create resistance. But in superconductors, all electrons behave as one, and individual defects do not prevent current from transmitting with virtually no resistance.

ORNL is a leader in investigations revealing similar extraordinary electronic behavior in quantum materials. Physicist Zac Ward and his research partners showed that complex materials subjected

to controlled electric and magnetic fields can self-organize into circuitry. Likewise, physicist Arnab Banerjee and colleagues observed quantum spin liquids, which preserve disorder even at very low temperatures, in two-dimensional magnets (see "Neutrons and quantum spin liquids," page 12).

Two-dimensional materials—that is, materials that tend to be just a few atoms thick—could make optoelectronic devices thinner and more energy efficient. For example, physicist An-Ping Li showed that changing the shape of a 2-D material alters how electrons connect and can turn a metal into an insulator.

It is not necessary that a material be 2-D to be a quantum material, although that is often the case. Solid-state physicist Brian Sales demonstrated a quantum critical point—where strong quantum mechanical fluctuations occur—in a structural alloy by controlling the concentration of magnetic dopants.

Scanning tunneling microscopy by materials scientists Sergei Kalinin and Peter Maksymovych and others reveals local electronic states. "That comes back to the very basic quantum levels," Christen said.

Meanwhile, solid-state chemist Athena Sefat (see "Fundamentally strong," page 6) leads a new program to explore the behavior of iron-based superconductors by synthesizing and measuring materials' bulk behavior



in single-crystal forms, combining theory with CNMS's electronic structure mapping capabilities. Simulations by condensed matter physicists Adriana Moreo and Elbio Dagotto clarified puzzling magnetic order in iron telluride. By examining how the spins interacted with the motion of the atoms, they theoretically reproduced the enigma.

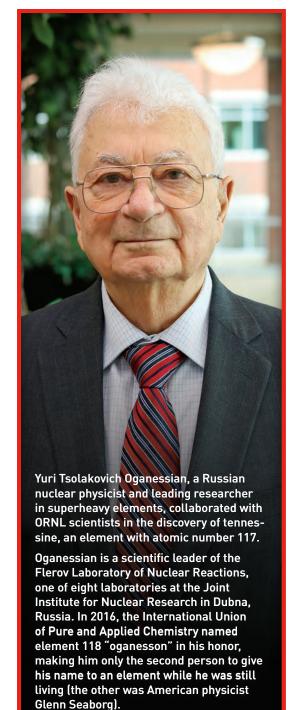
Materials scientists Ho Nyung Lee and Paul Snijders investigated these states in films that have been deposited

on a crystalline substrate. Moreover, Lee and physicist Mike Fitzsimmons layered transition metal oxides and showed exotic coupled magnetic behavior not observed in the component materials.

Transition metal oxides will be a testing ground for the Center for Predictive Simulation of Functional Materials, which DOE established in 2016 to accelerate the computer design of materials.

According to Paul Kent, the center's director, ORNL researchers will work with scientists from national labs and universities to develop software to accurately predict the properties of quantum materials. Kent also leads new efforts to continue the software development to take advantage of the next-generation computational capabilities of DOE's Exascale Computing Project. *

For more information: https:// go.usa.gov/xXxnQ



Oganessian delivered the Eugene Wigner Distinguished Lecture Jan. 27, 2017, on the topic "Discovering Superheavy Elements." This is an edited transcript of our conver-

sation following his lecture.

Distinguished

Yuri Tsolakovich Oganessian

- How did you first become interested in working with superheavy elements?

 After university I came to the Flerov group as a young physicist. Flerov was
 - a leading scientist in this field, and I started to think—like these people were thinking—about superheavy elements. When I started to understand more, after my education, I came to the conclusion that this really is a very exciting and interesting field, and I didn't change it.
- 2. Why is this work important?

First of all, it's important because it changes a little bit our understanding of the surrounding material world. Fifty years ago, at the time I started to work, we had a certain view about the limits of this work. The idea that there is a so-called island of stability proved this limit.

On the question of how many elements may exist, 50 years ago we would have said 100 only. We are now at 118 [oganesson], and we believe that we can move further.

3. How do international collaborations such as the one that produced tennessine help in the search for superheavy elements?

You can't make something significant in science alone. You have to take other cultures from different areas of the world and get them together, and then maybe you may succeed.

4. What can we expect in the future for superheavy element research?

That's a very good question. Here is a question which I ask my people: "We've done this research for 25 years, and we made it. If you start today to do the same things, how fast will you succeed?"

It's quite interesting. If you put in the one hand all you know about superheavy elements, and in the other hand you put all the progress which we have made in computer science, plasma physics, chemistry, computing and

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so on [areas that support superheavy element research]—if you put them together, what improvement factor can we get to make our research better [more sensitive]?

So in 15 years you may get a factor of 100. Based on such a statement, we decided to build a so-called superheavy element factory to get this factor of 100. A superheavy element factory is not a device; it's a collaboration. Oak Ridge may develop the reactors and develop new technologies for targets. We now are trying to build big, new accelerators which will have beams 10 times more intense. And together we are looking for new detectors, new separators—these are intellectual parts of the experiment. All this together will give us a factor of 100. And this will make us understand this new land of superheavy nuclei.

We don't know what they will look like, these superheavy nuclei and superheavy elements. But by understanding the properties, we may have a prediction for new, more heavy ones. We hope to have the first beam of a new accelerator at Dubna at the end of this year.

5. What role do you see for ORNL in this work?

The role of Oak Ridge is as a partner. We have to do it together. This is what collaboration is about. Otherwise I am not sure we can really have a result such as we have today.



The Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy gives scientists, business leaders and policy makers an opportunity to address the ORNL community and exchange ideas with lab researchers. The series is named after Eugene Wigner, ORNL's first research director and recipient of the 1963 Nobel Prize in Physics.









Batteries and fertilizer:

A conversation with ORNL chemist Gabriel Veith

RNL's Gabriel Veith is committed to saving energy through better batteries and more efficient chemical processes. He began pursuing his passions at the lab nearly 15 years ago, starting as a postdoc in the Materials Science and Technology Division.

In 2008 Veith earned an Early Career Award for Scientific Accomplishment from UT-Battelle for advances in nanoscale catalyst synthesis by new vapor deposition methods. He holds a PhD in inorganic chemistry from Rutgers University.

We talked with him about the importance of battery technology and the opportunities available for more efficient fertilizer production. This is an edited transcript of our conversation.

• What are you working on?

I'm an experimental chemist working on the synthesis and characterization of new materials for energy storage and conversion applications.

I focus on the development of thin film materials. An everyday example of a thin film would be the reflective coating on the inside of a potato chip bag. I also develop bulk powder materials. So I make materials from all different length scales and form factors.

I take these materials and use them in my experiments.

For example, I use thin films as model systems to study interfaces for batteries, collaborating with scientists at the Spallation Neutron Source. When we study the material as we charge and discharge it, we can follow how the interfacial chemistry evolves, which is important for battery life.

I also take powder materials and collaborate with microscopists here at ORNL, studying the structure and chemistry of these materials as a function of a catalytic reaction.

If we can understand these interfacial and structural changes and processes we can predict ways to control them which will enable improved performance of a battery or catalyst in the future.



What benefits will come from improving battery technology?

The obvious improvements in everybody's lives will be longer-lasting cellphones and vehicles that travel longer distances. For me, I think of improved batteries in terms of resiliency, energy security and reliability.

In the United States right now we produce a lot of renewable energy to produce electricity. The problem is you often produce electricity at times when you don't need the extra electricity or in places where you don't need to use it right then and there.

Traditionally we would use something called pumped hydro. When power plants are producing extra electricity they would pump water uphill, and when they needed extra electricity they would release the water from the dam through a turbine and generate electricity.

You can't use pumped hydro with something like solar energy because you're often in a desert or a place where water is scarce. You can't use pumped water in a place like Kansas, because there's not a significant elevation change to pump water up and have it go back down to generate electricity.



ORNL experimental chemist Gabriel Veith loads a deposition chamber to prepare battery samples. Image credit: Jason Richards

This points to the need to use something like batteries, where you can put a battery in a brownfield, or in a city, or under a bridge, and then you've got a place to store electricity so that you can use it when you need it.

This becomes important in rural locations such as where my mother lives or where my mother- and father-in-law live. There, when you lose electricity you no longer have the ability to pump water from your well to drink, take a shower, or flush the toilets. Also, you can lose electric heat. By having batteries that they can use in their home, they could store electricity for use when they lose power.

Batteries would also be important in extreme weather, like Super Storm Sandy in New Jersey or during the recent flooding in Louisiana, where it knocked out the power grid. If you were able to store electricity, this would aid the first responders and emergency medical teams and get the communities back up and running at a much faster pace.

You are also focused on new catalytic process. Why is this important?

Right now in the United States about 3 percent of our total energy consumption goes to the chemical reduction of nitrogen. This is taking nitrogen from the air and turning it into ammonia fertilizer. Now, 3 percent doesn't sound like a lot, but when you consider that there are only 200 factories worldwide for the reduction of nitrogen to make ammonia, this is a significant process in terms of energy for one chemical reaction.

We do this because it's the only way we have to make fertilizers right now, and without these fertilizers there would be mass starvation and death around the world. The amount of ammonia we need in the future is going to continue to grow as countries improve their economies, and people in those countries want higher protein diets. That will lead to a negative cycle where we need more and more ammonia.

I believe now is the time to improve these nitrogen reduction processes. This process that we're using now is over 100 years old. There have not been significant changes. But with the advances we've had in materials, chemistry, characterization and theory, now is the right time to reinvestigate these processes, develop new ways to do it, and rethink the whole nitrogen reduction cycle.

RNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished scientists and engineers, and put them to work at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

We asked some of these young researchers why they chose a career in science, what they are working on at ORNL, and where they would like to go with their careers.



Marissa E. Morales-Rodriguez

Graduate student, Energy and Transportation Science Division
Ph.D. student, Energy Sciences and Engineering, University of Tennessee (Bredesen Center)
Hometown: Toa Alta, Puerto Rico

What are you working on at ORNL?

During my tenure at ORNL I have worked on a number of projects related to sensors. These projects include sensing techniques using laser spectroscopy, using infrared quantum cascade lasers for standoff detection of chemicals. Last year, 2016, I joined a team of scientists developing sensors using printed electronics.

What would you like to do in your career?

I would like to keep developing new sensing techniques using additive manufacturing. The technology commercialization aspect of science is also an interest of mine. My goal is to develop new low-cost solutions for environmental monitoring and security applications that can change the way we detect chemical and physical parameters.

Why did you choose a career in science?

I believe science chose me. Originally I was going to be a flight attendant, as I wanted to travel the world. In school, I was encouraged to study science, and I did. Today, I continue to pursue science because continuously learning, discovering and working on new things is my passion.



Cole Andrew Gentry

Postdoc, Reactor and Nuclear Systems Division Ph.D., Nuclear Engineering, University of Tennessee Hometown: Chattanooga, Tennessee

What are you working on at ORNL?

I am currently working on the development and application of efficient high-fidelity neutronics simulation codes for both the current operating fleet of light water reactors and molten salt reactor design concepts.

What would you like to do in your career?

I would like to continue working on the advancement of reactor simulation capabilities, in regard to both efficiency and accuracy; but I would also like to contribute in some significant manner to the design and deployment of an advanced reactor concept.

Why did you choose a career in science?

I have always enjoyed working on intellectually stimulating problems, particularly those whose solution I feel may contribute significantly toward human progress. The field of science, of course, provides an essentially limitless number of such problems to indulge in.



Swaroop Pophale

Postdoc, Computer Science and Mathematics Division Ph.D., Computer Science, University of Houston, Houston, Texas Hometown: Mumbai, India

What are you working on at ORNL?

I am working on programming models research at ORNL. My primary focus is on OpenMP for on-node shared memory programming and Partitioned Global Address Space for internode programming. For both programming models, I identify new and helpful features and build prototypes.

What would you like to do in your career?

In the short term, I want to dig deep into the programming models world and gain expertise in the needs of the applications supported at ORNL. In the longer term, I hope to be a subject matter expert in programming models and focus more on hybrid programming.

Why did you choose a career in science?

From the very start I enjoyed science. Being ever curious, I always wanted to know why things were a certain way. Enjoyment and curiosity led to interest, and computer science just seemed like the natural next step.



Folami Alamudun

Postdoc, Computational Sciences and Engineering Division Ph.D., Computer Science, Texas A&M University Hometown: Owo, Ondo state, Nigeria

What are you working on at ORNL?

My work focuses on two areas: psychophysiology and natural language processing. The former involves biosensing devices for modeling humans to improve understanding and prediction of behavior. The latter work involves the development of machine learning tools to improve text understanding in the medical domain.

What would you like to do in vour career?

I have a deep interest in the use of computing technology not only to improve the way we work or accomplish tasks, but also to improve the person. This includes knowledge assimilation and cognitive and behavioral development, among other things.

Why did you choose a career in science?

Curiosity. Observing and understanding the world in which one exists gives one the power with which to shape and mold things for better or for worse. I am in favor of the former goal and have thus dedicated my life and career to doing just that.



Emily Clark

Graduate student, Fusion and Materials for Nuclear Systems Division Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center) Hometown: Morristown, TN

What are you working on at ORNL?

My research focuses on the thermal management challenge in the fusion community. Fusion reactions create a significant amount of heat, and the components must be cooled to survive. I perform computational fluid dynamics and thermal modeling of cooling components to inform and improve their design, thereby allowing for increased heat loads.

What would you like to do in your career?

I would like to continue to engage in a challenging, application-driven research career where I can tackle problems that will have an impact on our world. As part of my work, I hope to bridge the gap between the scientific community and the public through science communication and policy in order to help address our society's greatest challenges and foster the next generation of scientists.

Why did you choose a career in science?

I literally spent my childhood with my head in the clouds. My dad owns a small airplane, and I spent countless hours flying with him. I would often look out and ask questions about how flight or weather worked. Those experiences spurred my interest in science and led me to become an aerospace engineer.



Travis Lange

Graduate student, Consortium for the Advanced Simulation of Light Water Reactors Ph.D. student, Energy Sciences and Engineering, University of Tennessee (Bredesen Center) Hometown: LaCoste, Texas

What are you working on at ORNL?

I am applying the advanced modeling and simulation capabilities in CASL to investigate a particular problem in the nuclear power industry called "crud induced power shift." I am collaborating with industry partners to determine the value to industry of using these advanced tools in analyzing real world reactor designs.

What would you like to do in vour career?

My short-term goals are to continue working in research to increase my experience, and hone my skills in addressing and solving complex problems. Ultimately, I want to invent a meaningful advancement in the energy field and take that idea into commercial production and application to help support and improve the energy situation in the United States and maybe throughout the world.

Why did you choose a career in science?

I chose a career in science because I see it as a wonderful way to help people and improve their quality of life throughout the world. Technology and scientific knowledge, when it is applied in a positive way, can change the world for the better in wonderful and amazing ways, and I want to be an active part of that.

Liane Russell, pioneer of fetal rad safety

by Tim Gawne gawnetj@ornl.gov

oon after the dawn of nuclear science, scientists understood that exposure to ionizing radiation could be harmful, even if they were unsure how harmful. Marie Curie, the groundbreaking scientist who coined the term "radioactivity," most likely died from its effects eight years before the Manhattan Project was created.

The effort during World War II to create a self-sustaining nuclear chain reaction was accompanied by efforts to develop detectors, shielding and film badges to help scientists understand and reduce the risk. While physicists and chemists tend to get all the glory, there were teams of biologists embedded in the Manhattan Project, too, working to qualify and quantify the effects of radiation across a range of conditions.

After the war, ORNL—known then as Clinton Laboratories—moved to create a robust biology research program. First, however, it needed someone with one foot planted in biology and the other in this new field of "nucleonics." That person was Alexander Hollaender, who came to Oak Ridge from the National Institutes of Health. It was Hollaender who brought William and Liane Russell on board from Roscoe B. Jackson Memorial Laboratory in Maine.

Liane Russell had completed her course work at the University of Chicago but had yet to defend her dissertation, which focused on the critical stages of embryonic development during which radiation could have ill effects. It was a new consideration, and her investigation found correlations between embryonic exposure and physical birth defects.

After she defended her thesis in August 1949 and became Dr. Liane Russell, the couple continued to pursue the hazards of embryonic exposure to radiation at ORNL.

By mapping critical points of human gestation to the same points in mice, they concluded that the most critical period of gestation was between two and six weeks, when most women would not even know they were pregnant. Their recommendations weren't just for women working near a nuclear reactor, however. They also believed medical diagnostics such as X-ray imaging might harm a developing fetus.

In March 1952, the Russells published their recommendations in the journal *Radiology*. This publication led to the international



Liane and Bill Russell

guidance that pregnant women avoid radiological procedures and that women who might become pregnant restrict such procedures to two weeks after their last menstrual cycle. This was known as the "14-day rule."

While discussion of menstruation may have run counter to general sensibilities, the Russells also angered radiologists with the implication that accepted practice at that time may have been unsafe.

"These recommendations, published in 1952, brought the wrath of radiologists down upon our heads, and unleashed a series of letters to the editor," Liane Russell later wrote. "Before long, however, the so-called 14-day (sometimes 10-day) rule became internationally accepted in radiological practice."

Clearly the article had far-reaching effects. Today, any time you enter an area of a hospital or doctor's office where radiological imaging is taking place, you will be greeted by signs, questions and written materials insisting that you alert your doctor if you are pregnant or might become pregnant.



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Friday, May 6, 1949

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