OAK RIDGE NATIONAL LABORATORY

Review

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OAK RIDGE National Laboratory

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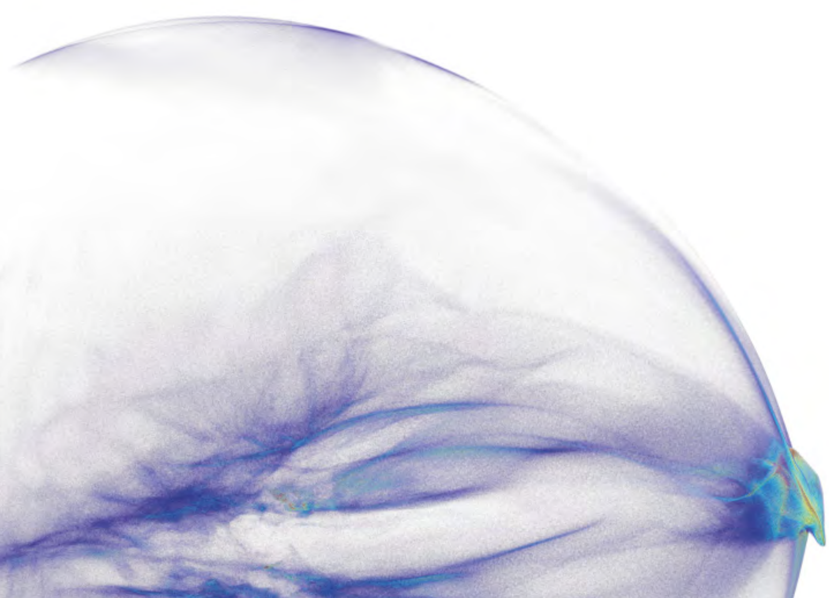


On the Cover

ORNL's Stan Wullschleger leads the NGEE Arctic project, which gathers data from Alaska's arctic region to incorporate into Earth system models. Image credit: Stan Wullschleger, ORNL

The amazing impact of ORNL isotopes

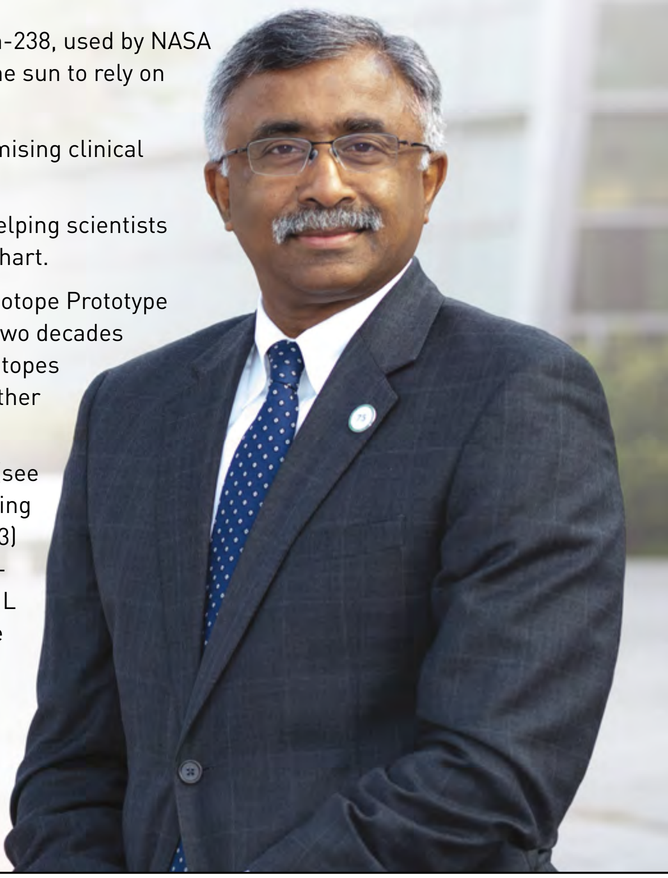
Isotopes—the variants of a chemical element—have benefited us in countless ways over the decades. They have extended our lives as cancer treatments, enhanced our security as radiation detectors, enabled deep space missions as power sources, and served as an indispensable element in research and manufacturing.

ORNL has been in the vanguard of isotope production since shortly after the lab was created in 1943. In 1946, Eugene Wigner, the lab's first director of research and development, made the first official delivery of a reactor-produced isotope—carbon-14—to the Barnard Free Skin and Cancer Hospital in St. Louis.

In the lab's early years, isotope production was handled by the Graphite Reactor—the world's first permanent nuclear reactor—and a group of facilities at ORNL's Isotope Circle. In the past 50-plus years, however, the lion's share of ORNL isotope production has been carried out at the High Flux Isotope Reactor and adjacent Radiochemical Engineering Development Center.

Consider the following:

- ORNL produces the majority of the world's californium-252, a versatile isotope that can detect impurities in coal and cement, calibrate radiation detection instruments in port security operations, and help start up dormant nuclear reactors.
- Since 2015, the lab has produced significant quantities of plutonium-238, used by NASA to power space missions that last too long and travel too far from the sun to rely on traditional batteries or solar power.
- ORNL is producing isotopes such as actinium-225 and -227 for promising clinical trials and FDA-approved drug applications for cancer treatment.
- Through the production of berkelium-249, ORNL was essential in helping scientists discover tennessine, the second-heaviest element on the periodic chart.



More recently, HFIR and REDC have been joined by the Enriched Stable Isotope Prototype Plant, created for DOE to restart U.S. production of stable isotopes after two decades of dormancy. These valuable isotopes are used as precursors for radioisotopes used in explosives detection and medical research and directly in many other critical applications.

In this issue of *ORNL Review*, we take a look at the lab's work in isotopes (see "Isotopes to the rescue," page 8). We delve into the promise offered by using isotopes to attack cancer cells (see "Radiation, meet cancer cell," page 13) and aid diagnostics (see "Made in the USA: Key isotopes for medical diagnostic imaging," page 15). We look at the critical work being done by ORNL staff to prepare very rare stable isotopes for research projects around the world (see "How do you want your isotope?" page 9). And we examine the lab's production of plutonium-238 to enable deep space explorations for years to come (see "ORNL on the red planet," page 11).

Isotope production has been a foundational ORNL capability throughout our long and rich history, and we are grateful for the opportunity to lead the way into the 21st century.

Thomas Zacharia

Thomas Zacharia
Laboratory Director

Three from ORNL become APS fellows

Three ORNL researchers have been elected fellows of the American Physical Society.

Gaute Hagen

Gaute Hagen, task leader of the Physics Division's Nuclear Theory program, was cited "for contributions to the development of coupled-cluster models in nuclear physics and his theoretical predictions for the structure of rare isotopes."

Masaaki Matsuda

Hagen's research with the Nuclear Theory group focuses on computational and theoretical advances in ab initio approaches for atomic nuclei, with the goal of understanding the structure and the decays of nuclei and the physics of matter at the extremes of the nuclear landscape.

Parans Paranthaman

Neutron scattering scientist **Masaaki Matsuda** was cited "for important contributions to the study of spin-lattice effects in frustrated magnets and to the study of electronic phase separation and magnetic excitations in lightly doped high-TC cuprate superconductors in using neutron scattering."

Matsuda is an instrument scientist on the Polarized Triple-Axis Spectrometer at ORNL's High Flux Isotope Reactor, where he researches magnetism in strongly correlated electron systems, quantum spin systems and multiferroic systems.

ORNL corporate fellow and Materials Chemistry Group leader **Parans Paranthaman** was cited "for distinguished contributions to the field of materials synthesis and characterization for high temperature superconductors, solar cells, lithium ion batteries and additive manufacturing of magnetic materials."

Paranthaman is a Distinguished UT-Battelle Inventor, 2016 ORNL Inventor of the Year and a UT-ORNL joint faculty member with the Bredesen Center for Interdisciplinary Research and Graduate Education.

APS fellows are recognized for their exceptional contributions to the physics enterprise in outstanding research, applications, and leadership in or service to physics and physics education. Each year, fewer than one-half of 1 percent of the society's members become APS fellows.—*Sean Simoneau*

Wireless vehicle charger rivals wired systems

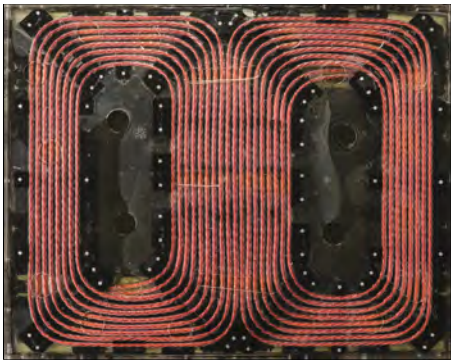
ORNL researchers have demonstrated a 120-kilowatt wireless charging system for vehicles—providing six times the power of previous ORNL technology and a big step toward charging times that rival the speed and convenience of a gas station fill-up.

The wireless system transfers 120 kilowatts of power with 97 percent efficiency, which is comparable to conventional, wired high-power fast chargers. In the laboratory demonstration, power was transferred across a 6-inch air gap between two magnetic coils and charged a battery pack.

ORNL researchers earlier created and demonstrated the world's first 20-kilowatt wireless charging system, which is being modified for applications such as commercial delivery trucks.

"It was important to maintain the same or smaller footprint as the previous demonstration to encourage commercial adoption," said project lead Veda Galigekere of ORNL's Power Electronics and Electric Machinery Group.

"We used finite element and circuit analyses to develop a novel co-optimization methodology, solving the issues of coil design while ensuring the system doesn't heat up or pose any safety issues and that any loss of power during the transfer is minimal," he said.



ORNL's unique wireless coils and power electronics are co-optimized to safely transfer large amounts of electricity across an air gap at 97 percent efficiency. Image credit: Genevieve Martin, ORNL

To achieve 120 kilowatts, the ORNL team created a new coil design co-optimized with the latest silicon carbide power electronic devices for a lightweight, compact system.

The system's architecture takes energy from the grid and converts it to high-frequency alternating current, which generates a magnetic field that transfers power across a large air gap. Once the energy is transferred to the secondary coil, it is converted back to direct current and stored in a vehicle's batteries.—*Kim Askey*

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

Accelerator beam measured in 6D

The first full characterization measurement of an accelerator beam in six dimensions will advance the understanding and performance of current and planned accelerators around the world.

A team of researchers led by the University of Tennessee, Knoxville, conducted the measurement in a beam test facility at ORNL using a replica of the Spallation Neutron Source's linear accelerator, or linac. The details are published in the journal *Physical Review Letters*.

"Our goal is to better understand the physics of the beam so that we can improve how accelerators operate," said Sarah Cousineau, group leader in ORNL's Research Accelerator Division and UT joint faculty professor. "Part of that is related to being able to fully characterize or measure a beam in 6D space—and that's something that, until now, has never been done."

Six-dimensional space is like 3D space but includes three additional coordinates on the x, y and z axes to track motion or velocity.

"Right away we saw the beam has this complex structure in 6D space that you can't see below 5D—layers and layers of complexities that can't be detangled," Cousineau said. "The measurement also revealed the beam structure is directly related to the beam's intensity, which gets more complex as the intensity increases."

Previous attempts to fully characterize an accelerator beam fell victim to "the curse of dimensionality," in which measurements in low dimensions become exponentially more difficult in higher dimensions. Scientists have tried to circumvent the issue by adding three 2D measurements together to create a quasi-6D representation. The UT-ORNL team notes that approach is incomplete as a measurement of the beam's initial conditions entering the accelerator, which determine beam behavior farther down the linac.—*Jeremy Rumsey*

This artistic representation illustrates a measurement of a beam in a particle accelerator, demonstrating that the beam's structural complexity increases when measured in progressively higher dimensions. Image credit: Jill Hemman, ORNL

ORNL geospatial data aids disaster relief

As hurricanes barrel toward the coastlines and wildfires rage in arid regions of the United States, ORNL scientists are providing critical geospatial data to support first responders as they work to save lives and property.

To assist FEMA with the Carr Fire emergency response in California, ORNL researchers used satellite images and novel computing techniques to rapidly identify and deliver data of nearly 97,000 potentially impacted or vulnerable homes and buildings in Shasta and Trinity counties. Image credit: Melanie Laverdiere, ORNL

When disasters strike, many homes and buildings succumb to winds, floods or flames. To assist humanitarian and damage assessment efforts, ORNL researchers are using novel computing techniques to rapidly identify structures on the ground from satellite images or determine where the structures once stood.

Behind the scenes, the geographic information team digitally sifts through thousands of images and collects meaningful data in a matter of hours, a process that previously would take several months.

"When you look at imagery such as what's shown in Google Maps, it's very easy to visually distinguish what is a building and what is not," said Melanie Laverdiere, a geographic information system scientist at ORNL. "However, extracting this meaningful information in an automated fashion into a tangible data set is much more complex."

Laverdiere works with ORNL project team lead Mark Tuttle and colleagues who are actively supporting the Federal Emergency Management Agency, or FEMA, with information on buildings and structures in a hurricane's path and those that remain in harm's way. Their technique was also applied for California's Shasta and Trinity counties, both affected by the recent Carr Fire.

The team collects large sets of data that identify and characterize hundreds of vulnerable and affected structures, such as residences, businesses, schools and hospitals. This information proves critical to FEMA—the agency responsible for directing emergency response and assessing damages after an emergency event to inform recovery operations.—*Sara Shoemaker and Ashley Huff*

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

Kropaczek named new CASL director

The Consortium for Advanced Simulation of Light Water Reactors at ORNL has named David J. Kropaczek its director.

David J. Kropaczek

CASL, which launched in 2010 as DOE's first Energy Innovation Hub, has brought together the nation's supercomputing facilities and leading nuclear experts and institutions to pursue an aggressive 10-year mission—to predict the performance of existing and next-generation commercial nuclear reactors through comprehensive, science-based modeling and simulation.

"David is well equipped to lead CASL into this next stage. The program's innovative modeling tools have shown great promise, and it's time to hand the keys over to industry to ensure the greatest impact," said Alan Icenhour, associate laboratory director for the Nuclear Science and Engineering Directorate at ORNL. "Because of David's two decades of industry leadership experience and knowledge of CASL's inner workings, he is the right choice to push the program forward."

Kropaczek has served as chief scientist of CASL since 2016, interacting with CASL's science and industry councils and using their input to help shape the overall direction of the program's research. He has also represented CASL during technical meetings with DOE, which included coordinating and planning with related nuclear programs.

"As CASL enters the last phase under its 10-year directive, I'm excited to take the reins and lead the deployment of our tools to industry, specifically the Virtual Environment for Reactor Applications suite," Kropaczek said. "We want to realize the full value of CASL's impact by helping to safely extend the lifetime of the current nuclear fleet and assist industry in launching the next generation of nuclear reactors."—*Jason Ellis*

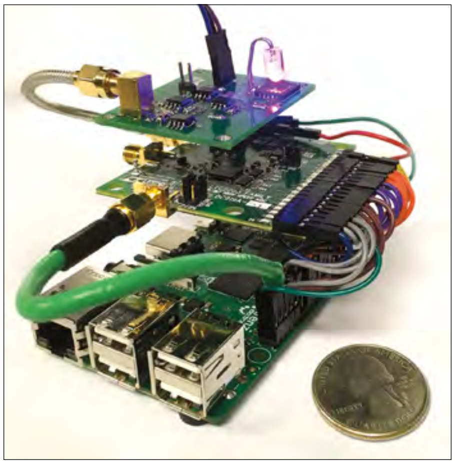
For more information: https://go.usa.gov/xPdvX

ORNL tech protects against cyberattacks

Qrypt Inc. has exclusively licensed a novel cybersecurity technology from ORNL, promising a stronger defense against cyberattacks including those posed by quantum computing.

Qrypt will incorporate ORNL's quantum random number generator, or QRNG, into the company's existing encryption platform, using inherent quantum randomness to create unique and unpredictable encryption keys enabling virtually impenetrable communications.

The advent of quantum computing offers a fundamentally new approach to solving some of the world's most difficult and pressing problems. However, quantum computing will also render current encryption methods obsolete and require a reimagined, quantum-based approach to protecting data.



ORNL's quantum random number generator began with basic components including an LED light from which a field of quadrillions of photons is produced. The device can detect and measure the quantum statistics of photons present in the field and use each one as the basis for creating truly unique encryption keys that are impossible to decipher or predict.
Image credit: Brian Williams, ORNL

"The cryptography we have developed is based on true quantum sources of entropy and is mathematically proven to be unbreakable—even in theory," said Denis Mandich, Qrypt's chief technology officer at the company's New York City office.

"Until recently, this class of technology was unavailable at the scale required to encrypt Internet-sized datasets," Mandich said. "Simply relying on increasing the complexity of cryptographic algorithms has again proven to be a failing bet."

ORNL's research is integral to Qrypt's hybrid approach: combining quantum physics hardware with post-quantum cryptographic algorithms and software. "We anticipate a long and productive partnership with one of the nation's premier labs as we continue to develop secure computing technologies," Mandich added.

One method for successful, fail-safe encryption will come from encoding messages with encryption keys that are truly random. That is, there is no realistic chance the exact key sequence used could be generated more than once.

To harness quantum's perfect randomness, ORNL coinventor Raphael Pooser and his colleagues from the lab's quantum sensing, computing and communications teams developed a quantum random number generator that detects the presence and characteristics of electromagnetic waves, called photons, streaming from a light source.—*Sara Shoemaker*

For more information: https://go.usa.gov/xPd6j

Cannibalized material forms new structures

ORNL scientists have induced a two-dimensional material to cannibalize itself for atomic "building blocks" from which stable structures formed.

The findings, reported in *Nature Communications*, provide insights that may improve the design of 2D materials for fast-charging energy-storage and electronic devices.

"Under our experimental conditions, titanium and carbon atoms can spontaneously form an atomically thin layer of 2D transition-metal carbide, which was never observed before," ORNL's Xiahan Sang said.

He and ORNL's Raymond Unocic led a team that performed *in situ* experiments using state-of-the-art scanning transmission electron microscopy, combined with theory-based simulations, to reveal the mechanism's atomistic details.

"This study is about determining the atomic-level mechanisms and kinetics that are responsible for forming new structures of a 2D transition-metal carbide such that new synthesis methods can be realized for this class of materials," Unocic added.

The starting material was a 2D ceramic called a MXene (pronounced "max een"). Unlike most ceramics, MXenes are good electrical conductors because they are made from alternating atomic layers of carbon or nitrogen sandwiched within transition metals like titanium.

The research was a project of the Fluid Interface Reactions, Structures and Transport Center, a DOE Energy Frontier Research Center that explores fluid–solid interface reactions that have consequences for energy transport in everyday applications.

The high-quality material used in these experiments was synthesized by Drexel University scientists, in the form of five-ply single-crystal monolayer flakes of MXene. The flakes were taken from a parent crystal called "MAX," which contains a transition metal, denoted by "M"; an element such as aluminum or silicon, denoted by "A"; and either a carbon or nitrogen atom, denoted by "X." The researchers used an acidic solution to etch out the monoatomic aluminum layers, exfoliate the material and delaminate it into individual monolayers of a titanium carbide MXene.—*Dawn Levy*

For more information: https://go.usa.gov/xPdv2

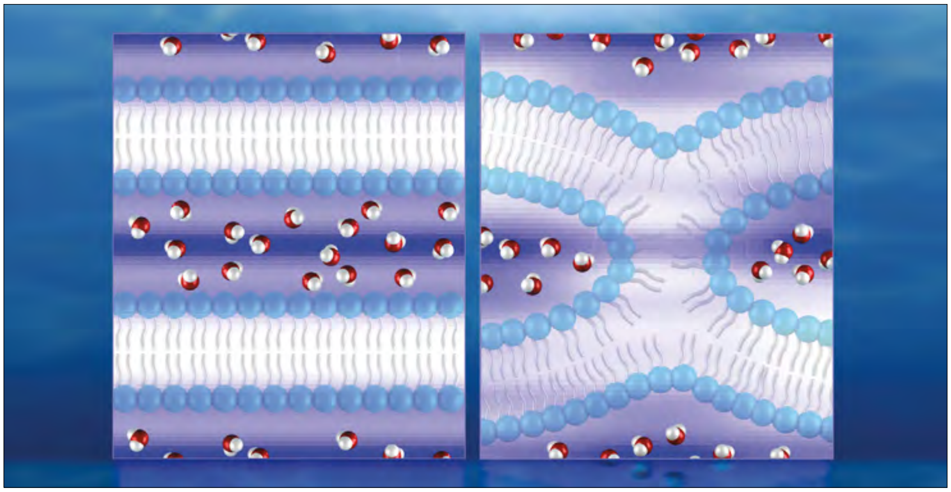


Illustration of neutron diffraction data showing water distribution (red-and-white molecules) near lipid bilayers prior to fusion (left) and during fusion. Mapping the water molecules is key to understanding the process of cell membrane fusion, which could help facilitate the development of treatments for diseases associated with cell fusion. Image credit: ORNL

Neutrons illuminate cell development

New 3D maps of water distribution during cellular membrane fusion are accelerating scientific understanding of cell development, which could lead to new treatments for diseases associated with cell fusion.

Using neutron diffraction at ORNL's Spallation Neutron Source and High Flux Isotope Reactor, researchers have made the first direct observations of water in lipid bilayers used to model cell membrane fusion.

The research, published in the *Journal of Physical Chemistry Letters*, could provide new insights into diseases in which normal cell fusion is disrupted, such as Albers-Schönberg disease (osteopetrosis). It could also help facilitate the development of fusion-based cell therapies for degenerative diseases and lead to treatments that prevent cell-to-cell fusion between cancer cells and noncancer cells.

"We used neutrons to probe our samples because water typically can't be seen by X-rays and because other imaging techniques can't accurately capture the extremely rapid and dynamic process of cellular fusion," said Durgesh K. Rai, coauthor and now a postdoctoral researcher at Cornell University.

The researchers' water density map indicates the water dissociates from the lipid surfaces in the initial lamellar, or layered, phase. In the intermediate fusion phase, known as hemifusion, the water is significantly reduced and squeezed into pockets around a stalk—a highly curved lipid "bridge" connecting two membranes before fusion fully occurs.—*Paul Boisvert*

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

Math explains challenges of poor neighborhoods

New mathematical models developed by ORNL with collaborators at Sam Houston State University and the University of Chicago can help guide changes to the layout of poor urban neighborhoods to improve access to resources with minimum disruption and cost.

The researchers established a novel way to mathematically analyze poor and informally developed urban communities, revealing obstacles between unplanned areas and the infrastructure that provides resources for basic human necessities. In their paper published in *Science Advances*, they used satellite imagery and municipal data to develop mathematical algorithms that reveal that slums and planned neighborhoods are fundamentally different.

Their models clearly identify distinctions between the informal arrangement of underserviced urban areas and the formal structure of city neighborhoods. In two case studies, the researchers used real-world data to show that the physical layout of some unplanned neighborhoods does not allow space for sewer lines, roads or water pipes.

Of the estimated 4 billion people currently living in urban areas worldwide, approximately 1 billion reside in slums. With inadequate infrastructure for health, sanitation and access to emergency services, these areas face humanitarian and sustainability issues in the wake of rapid urbanization. Christa Brelsford, an ORNL Liane Russell Fellow and lead author, believes this research can transform the future of slums.

"For me, this research was an opportunity to look at cities from a new and exciting mathematical perspective," Brelsford said. "By putting these tools in the hands of local community organizations and residents, efforts for accessible infrastructure empower residents to make decisions about their neighborhoods and communities."

"Anything we can do to improve lives from a human rights perspective is both good for the world and also supports U.S. national security, because the more people have their basic needs met, the more secure we all are," she added.—*Shelby Whitehead*

This graphic of a South African neighborhood is overlaid with colors that indicate the number of obstacles between a home and access to resources. Image credit: Christa Brelsford, ORNL, and Luis Bettencourt, University of Chicago

Four ORNL researchers become AAAS fellows

Four ORNL researchers have been elected fellows of the American Association for the Advancement of Science.

AAAS is the world's largest multidisciplinary scientific society and publisher of the *Science* family of journals. ORNL's four fellows join a class of 416 members awarded the honor this year by AAAS for their "scientifically or socially distinguished efforts to advance science or its applications."

Phillip F. Britt, director of the Chemical Sciences Division, was elected by AAAS Chemistry Section for "distinguished contributions in the field of fuel chemistry, service to the chemistry profession and leadership of a world-class research organization."

Britt joined ORNL in 1988 as a physical organic chemist and has led the lab's Chemical Sciences Division since 2006. He is a highly published author and a fellow of the American Chemical Society, and he received the Secretary of Energy's Achievement Award in 2015. He is also on the Board of Visitors for the Department of Chemistry at the University of Tennessee.

Stephan Irle, computational soft matter scientist in the Computational Sciences and Engineering Division and the Chemical Sciences Division, was elected by the AAAS Chemistry Section for "distinguished contributions to the field of computational chemistry, particularly for modeling and predictions of electronic and molecular structure and complex systems dynamics."

Phillip F. Britt

Stephan Irle

Bruce Moyer

Amy Wolfe

Before joining ORNL in 2017, Irle was a professor of chemistry and a founding principal investigator of the Institute of Transformative Bio-Molecules at Nagoya University in Japan. He was a member of the Japanese "K supercomputer" support project and specializes in the quantum chemical study of complex systems, including soft matter and biosimulations, excited states of large molecules, catalysis and geosciences.

Bruce Moyer, leader of the Chemical Separations Group in the Chemical Sciences Division, was elected by the AAAS Chemistry Section for "exemplary service, research and technology development in the field of separation science and technology benefiting the environment, nuclear energy and critical materials."

Moyer is an ORNL Corporate Fellow with nearly 40 years of experience in separation science and technology, especially in applying fundamental principles to waste treatment, nuclear fuel recycling and the recovery of critical materials. Moyer led the chemical development of the caustic-side solvent extraction process used in the cleanup of millions of gallons of high-level radioactive waste at the Savannah River Site, which earned him multiple awards, including the Secretary of Energy's Achievement Award.

Amy Wolfe, leader of the Society, Energy and Environment Group in the Environmental Sciences Division, was elected by the AAAS Societal Impacts of Science and Engineering Section for "distinguished achievements in quality, visibility and application of social science research on the science and technology enterprise within the U.S. national laboratories and beyond."

Wolfe has studied the social, institutional and behavioral intersections of society and technology and led several research groups since joining ORNL in 1985. She serves on the AAAS Committee on Scientific Freedom and Responsibility, was a program committee member for the Behavior, Energy and Climate Change Conference, and has represented ORNL in several multilaboratory efforts for the Department of Defense and DOE's Office of Energy Efficiency and Renewable Energy.—*Sean Simoneau*

Experiment opens stage for discovery on matter

If equal amounts of matter and antimatter had formed in the Big Bang, they would have annihilated each other upon meeting, and today's universe would be full of energy—but no matter to form stars, planets and life.

Yet matter exists now. That fact suggests something is wrong with Standard Model equations describing symmetry between subatomic particles and their antiparticles.

"The excess of matter over antimatter is one of the most compelling mysteries in science," said John Wilkerson of ORNL and the University of North Carolina, Chapel Hill. He leads the MAJORANA Demonstrator experiment, in which 129 researchers from 27 institutions and six nations investigate the nature of neutrinos. These electrically neutral particles interact only weakly with matter, making their detection exceedingly difficult.

The MAJORANA Demonstrator's key accomplishment, published in March 2018, was showing it was possible to avoid background from cosmic rays and radioactivity that could mimic the signal of a phenomenon that has never been observed, called "neutrinoless double-beta decay." Its observation would demonstrate that neutrinos are their own antiparticles and have profound implications for our understanding of the universe.

"It's critical to know that radioactive background is not going to overwhelm the signal you seek," said ORNL's David Radford, a lead scientist in the experiment.

The researchers shielded a sensitive, scalable 44-kilogram germanium detector array from background radioactivity. This accomplishment is critical to developing and proposing a much larger future experiment—with approximately a ton of detectors—seeking the signal of neutrinoless double-beta decay.

Researchers work on the delicate wiring of a cryostat, which is like a thermos under vacuum and chills the detectors that are the heart of the MAJORANA Demonstrator. Image credit: Matthew Kapust, Sanford Underground Research Facility

Siting the MAJORANA Demonstrator under nearly a mile of rock at the Sanford Underground Research Facility in South Dakota was the first of many steps collaborators took to reduce interference from background. Other steps included using a cryostat made of the world's purest copper and a complex six-layer shield to eliminate interference from cosmic rays, radon, dust, fingerprints and naturally occurring radioactive isotopes.—*Dawn Levy*

For more information: https://go.usa.gov/xUH4Q

Summit helps teams win supercomputing award

Two DOE national laboratories have been awarded the 2018 Association for Computing Machinery's Gordon Bell Prize for work done on ORNL's Summit supercomputer, the most powerful system in the world.

Winners of the prize, which recognizes outstanding achievement in high-performance computing, were announced November 15 during the 2018 International Conference for High Performance Computing, Networking, Storage, and Analysis in Dallas.

One of the winners, a team co-led by ORNL computational systems biologist Dan Jacobson and computational scientist Wayne Joubert, is leveraging population-scale genomic datasets and algorithmic advances to uncover hidden networks of genes at incredible speeds.

The team developed a genomics algorithm capable of using mixed-precision arithmetic to attain exaops speeds, or greater than a billion billion calculations per second.

The ORNL-led team shared this year's Gordon Bell prize with a team led by computational scientists and engineers from Lawrence Berkeley National Laboratory, ORNL and Nvidia; that team was recognized for applying a deep-learning application to extreme climate data and breaking the exaop barrier for the first time with a deep-learning application.

The team used Summit to apply deep-learning methods to extract detailed information from climate data produced at the National Energy Research Scientific Computing Center. Rather than computing simple quantities such as average global temperature, these methods discover and locate features like hurricanes and atmospheric rivers, which are important in characterizing extreme weather patterns and their impact.—*Katie Bethea*

Genetic shortcoming found for poplar vulnerability

Scientists studying a valuable, but vulnerable, species of poplar have identified the genetic mechanism responsible for the species' inability to resist a pervasive and deadly disease. Their finding, published in the *Proceedings of the National Academy of Sciences*, could lead to more successful hybrid poplar varieties for increased biofuels and forestry production and protect native trees against infection.

A research team—jointly led by ORNL and Oregon State University in partnership with the DOE Joint Genome Institute and the University of Georgia—analyzed the genetic response of purebred black cottonwood poplars infected by a pathogen known as Septoria.

Septoria causes untreatable cankers, or wounds, on the surface of the trunk and branches and kills trees early in the growing cycle.

"Since the 1900s, industry has tried to grow hybrid varieties of poplar—including those made by crossing eastern cottonwood and black cottonwood—to produce a faster-growing tree, and they have been puzzled by the early death of hybridized poplars grown in many parts of the United States," said Wellington Muchero, a researcher with the Center for Bioenergy Innovation at ORNL and the study's lead author.

Hybrid varieties are economically valuable because they can grow up to three times faster than the pure species. If the hybridized poplars survive, they could dramatically increase production of high-value, bioderived materials, biofuels and forestry products such as pulp and paper, lumber and veneer.

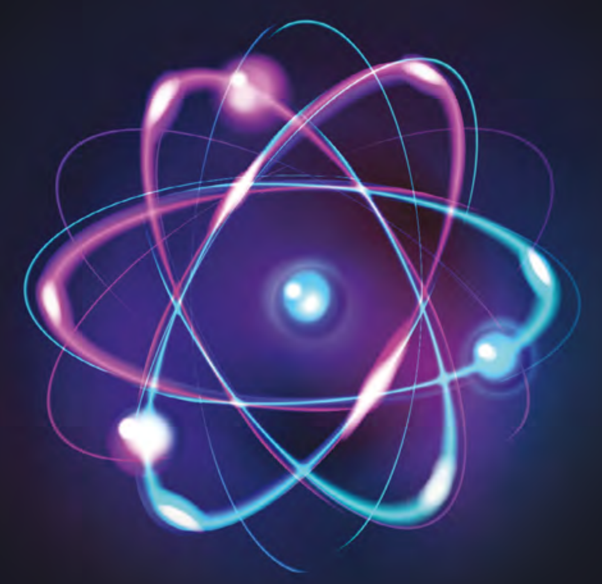
Black cottonwood poplars grow natively in river systems across the Pacific Northwest region of the United States where Septoria is not yet a threat.

"What our study revealed is a double whammy for black cottonwoods," said Muchero, a specialist in plant microbe interfaces. "Since the pathogen is not prevalent in its native region, these trees have allowed their genetic resistance mechanisms to fall apart with no consequence."—*Sara Shoemaker*

For more information: https://go.usa.gov/xPzh6

Scientists have found the genetic mechanism behind the early death of certain varieties of poplar trees. Their finding could lead to more successful, fast-growing hybrid poplars for increased biofuels and forestry production and protect native trees against infection. Image credit: Jay Chen, ORNL

Isotopes to the rescue



by Leo Williams
williamsjl2@ornl.gov

Men with prostate cancer that has spread to their bones can get some relief from a radioactive isotope of radium.

Radium-223, marketed by Bayer as Xofigo, attacks cancerous growths in bones, helping to reduce painful fractures and potentially extending a sufferer's life.

This valuable treatment owes its effectiveness to two characteristics of radium-223. First, the element radium is chemically similar to calcium, so radium introduced into the body goes straight to the site of growing bone—in this case a growing cancer. Second, the isotope radium-223 emits alpha radiation, which gives off a lot of energy over a very short distance—in this case, a diameter of about a ten-thousandth of a meter, or about 10 cells. As a result, it is largely able to kill cancer cells while leaving other cells unharmed.

The treatment has been approved in the United States since 2013 and, as of 2018, its radioactive essence comes from ORNL's High Flux Isotope Reactor.

ORNL is a major source of isotopes, providing more than 300 for use in medicine, research, industry and space exploration. Many are or can be produced at lab facilities such as HFIR, the Radiochemical Engineering Development Center and the Enriched Stable Isotope Prototype Plant.

"The isotopes provide capabilities that don't exist without them," explained Kevin Hart, manager of ORNL's isotopes program. "In some cases, we are making isotopes that don't exist in nature—they would not be there unless we made them."

What is an isotope?

Elements and isotopes are determined by the number of particles in an atom's nucleus. The element itself is defined by the number of positively charged protons, so that an atom with one proton is hydrogen, one with six protons is carbon, one with 92 is uranium, and so on. Scientists have identified or created 118 elements, from hydrogen up to oganesson, which has 118 protons.

The isotope, on the other hand, is determined by the number of uncharged neutrons in the nucleus. While all carbon atoms have six protons, they can have anywhere from two to 16 neutrons. If they have eight neutrons, for instance, they are carbon-14 (the total number of protons plus neutrons) and can be used for carbon dating.

There are two primary ways ORNL creates isotopes, depending on whether they are radioactive or stable. For radioactive isotopes, HFIR creates new elements and isotopes by bombarding a target

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How do you want your isotope?

by Leo Williams
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ORNL materials processing researcher Mike Zach. Image credit: Carlos Jones, ORNL

Stable isotopes require expert handling before they go to end users.

A researcher ordering an isotope may need it in any one of a wide variety of forms, such as a tiny foil, a coin-sized plate, a short wire, or a cylinder made to excruciatingly precise specifications.

Converting an isotope from a powder to that final form is an intensive, multi-stage process that may require specialized equipment, high temperatures, highly toxic and corrosive chemicals, oxygen-free environments and days of laborious manipulation.

And, to make the job even more of a challenge, the isotope itself is likely to be extremely precious. The rarest of these isotopes, once they have gone through a very specialized enrichment process, are far more valuable than gold.

Under the circumstances, then, it's no wonder that researchers want them delivered ready to use rather than having to fabricate the isotopes themselves.

That's where ORNL's Stable Isotope Group comes in. Experts in the group use extensive knowledge and specialized equipment to fabricate stable isotopes, ensuring these enormously valuable resources are used with minimal waste.

"My job is to take and transform any of the enriched stable isotopes into whatever form a researcher needs to make their project successful," said ORNL materials processing researcher Mike Zach. "That can entail making thin films, wires or special little forms, or they may need us to press it into a cylinder that is very exacting—within 20 microns in diameter and length, for instance, and within 99.5 percent of the theoretical density.

"I will work with the researchers to figure out what their experiment requires, then I've got to figure out how to do it."

The current inventory of stable isotopes was created in the calutrons at the Y-12 nuclear weapons plant near ORNL, but the calutron facility was shut down in 1998. New facilities are under development at ORNL to get American production of stable isotopes back up to speed; at most, only a few grams of most isotopes will be produced per year.

As a result, there will still be little room for waste, and researchers from around the world will still need Zach and his ORNL colleague Eva Hickman to make these materials into their final form. From ORNL's labs, they go to researchers in areas such as medical research, national security and fundamental science.

The materials are stored in a variety of chemical forms—oxides, fluorides and metals—and working with them often means converting those chemical forms.

So if, for example, the isotope is a rare earth metal oxide, Zach or Hickman must make it react with highly corrosive, highly toxic hydrogen fluoride gas, heating it to more than 700 degrees Celsius—or nearly 1,300 degrees Fahrenheit. Once it is converted to a fluoride, a second chemical reaction uses calcium metal at over 1,000 degrees Celsius (more than 1,800 degrees Fahrenheit) to remove

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Julie Ezold, manager for the californium-252 program at ORNL. Image credit: Carlos Jones, ORNL

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material with neutrons to increase the number of both protons and neutrons in the nucleus.

HFIR is supported by the nearby Radiochemical Engineering Development Center. Facilities at the center, including research laboratories, heavily shielded hot cells and glove boxes, are able both to create new targets for HFIR and to harvest newly created isotopes from targets that come out of the reactor.

For stable isotopes, facilities at the Enriched Stable Isotope Prototype Plant, or ESIPP, separate the different isotopes already present in a material, thereby enriching—or increasing the concentration of—a desired isotope.

The two types of isotope—radioactive and stable—go through very different production processes.

"The radioisotopes require controls like hot cells and glove boxes and lots of containment and highly regulated quantities and packaging," Hart said. "On the other hand, I can have a bottle of stable isotopes right on my bench top, because there's no decay particles, there's no hazards other than the chemical hazard of whatever formulation the chemical takes—so it would be like any other chemical that we might have here at the lab."

Making isotopes with neutrons

The creation of isotopes at HFIR involves two processes in the nucleus, explained Julie Ezold, manager for the californium-252 program at ORNL.

The first is neutron capture. HFIR is called "high flux" for a reason: The reactor shoots as many as 2 million billion neutrons each second through a space smaller than the face of a dime. On occasion, one of those neutrons is absorbed by an atom's nucleus, changing the isotope.

The second process is called "beta decay." In it, one of the neutrons becomes a proton—changing the element—and the atom spits out an electron and an antineutrino.

To produce californium, for instance, you start with targets made of curium, which has 96 protons and anywhere from 148 to 152 neutrons (curium-244 to curium-248). As they are bombarded, the nuclei slowly take on neutrons.

Unfortunately, most immediately split apart. In fact, 90 percent of nuclei that transform from curium-245 to -246 are lost through this process, known as fission. The nuclei that don't split apart

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ORNL on the red planet

by Leo Williams
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The car-sized Mars 2020 rover will be noteworthy for a variety of reasons. It will be on the lookout for evidence that the red planet once supported microbes. It will test a method for producing oxygen from the Martian atmosphere. And it will be the first NASA mission to contain plutonium produced at ORNL.

NASA uses plutonium—specifically the isotope plutonium-238—to power its space explorations. Specialized generators take heat produced by the isotope's radioactive decay and turn it into electricity to power faraway missions. With a half-life of nearly 88 years, Pu-238 is an excellent long-term source of power. It outlasts chemical fuel and, unlike solar power, it doesn't wane as a mission speeds away from the sun.

The United States lost its ability to produce Pu-238 when the Savannah River Site's K Reactor in South Carolina shut down in 1988. That loss and our shrinking inventory of the space-powering isotope fueled concern that the lack of plutonium-238 could stifle NASA's ability to do its job.

In response, DOE has been ramping up a collaboration with Idaho and Los Alamos national laboratories to replace the nation's supply of Pu-238. The heart of that effort lies in the abilities of two ORNL facilities: HFIR and the adjacent Radiochemical Engineering Development Center. REDC, which is equipped with hot cells, takes neptunium oxide provided by Idaho National Laboratory and turns it into pellets, which are assembled into targets that are loaded into HFIR. HFIR bombards the targets with neutrons, causing neptunium atoms to become plutonium atoms. And REDC then runs the targets through a chemical separation process to isolate the plutonium and recycle the unused neptunium.

The program, aimed at producing 1.5 kilograms of plutonium each year, is well on its way, having completed three production campaigns. The third, which was completed in early 2018, recovered about 250 grams of new plutonium. The material needed to be relatively free of other radioactive materials such as uranium, thorium and neptunium, as well as chemicals such as zinc, boron and phosphorous. The plutonium content also needed to be better than 82 percent Pu-238. The ORNL plutonium easily met those requirements, and in fact came in at 86 to 88 percent Pu-238.

"We nailed it really," said Pu-238 Supply Program Manager Bob Wham. "We did a really good job of getting it cleaned up. What we gave them was as good as they would use in a fuel clad. So we beat our own requirements by maybe an order of magnitude."

NASA seems pleased as well. A recent review from the National Academies said, "The PSD [NASA Planetary Science Division] has made dramatic progress in reestablishing a viable production source for Pu- 238. NASA and DoE have established a long-term relationship where NASA will fund the establishment and maintenance of a constant production line for Pu-238. This arrangement will reduce mission risk by maintaining a qualified work force and making targeted equipment investments across the production chain."

Generators on the Mars 2020 rover will contain a mix of plutonium from the Savannah River Site and ORNL, Wham said.

NASA's Mars 2020 Rover artist's concept. Image credit: NASA/JPL-Caltech

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gradually move through the transmutation process by adding neutrons until they become curium-249.

Curium-249 has a half-life of one hour, transforming into berkelium, which has 97 protons. The process continues until the berkelium transforms into californium, with 98 protons. Then you add neutrons until you get to your goal, californium-252.

Californium-252 is a neutron emitter with a variety of uses. It is used to start up nuclear reactors and is very useful for analyzing anything from coal and minerals to nuclear fuel rods. It can also help identify oil in an oil well.

> *"One of the drivers is to ensure that researchers in the United States have access to a domestic source of enriched stable isotopes, because foreign manufacturers may or may not be producing isotopes the researchers need."*
>
> — ORNL's isotopes program manager **Kevin Hart**

To produce californium, the targets stay in the reactor through four 24-day cycles. The time depends on the characteristics of the isotope and the number of neutrons a nucleus needs to absorb. Other processes can be longer or shorter; nickel-62 is very resistant to neutron capture, so those targets are left in the reactor for nearly two years to add one neutron to enough nuclei, transforming them to nickel-63, which is valuable for detecting explosives.

HFIR is not used exclusively for isotope production, Ezold noted. In fact, its most prominent use is in cutting-edge neutron scattering research—the use of neutrons to probe the atomic behavior of material and biological systems. Even so, isotope production at the reactor is very important.

"The 'I' in HFIR has always been for isotopes," Ezold said, "Having these facilities, both the reactor and the hot cell facilities, is unique in the world."

Separations at ESIPP

Most of the American inventory of stable isotopes was enriched in calutrons at Oak Ridge's Y-12 nuclear weapons plant. The calutrons were specialized mass spectrometers built during World War II to enrich uranium for nuclear weapons, and while most were decommissioned after the war, from eight to 16 were kept in production until 1998 to enrich other isotopes.

To restart American isotope production, DOE agreed in 2009 to build a new facility at ORNL. The prototype electromagnetic isotope separator—or EMIS—was commissioned in 2011. At the time it had about 10 percent of the output of a calutron, but upgrades completed in 2016 made it equivalent to a calutron in output.

The process used by the EMIS relies on the fact that each isotope of an element has a different mass.

First, the element is converted into a gas that is then ionized. Because ions are electrically charged, a stream of them bends as it passes through a magnetic field, but not all the ions bend by the same amount. The isotopes have different masses, and the lighter ones change direction more than the heavier ones.

The result is multiple beams, each containing a single isotope pointed at a collection pocket lined with graphite.

To date, the biggest achievement for the EMIS was production of 350 milligrams of ruthenium-96 for a physics experiment at Brookhaven National Laboratory. That project earned the ORNL team a DOE Secretary's Honor Award.

The EMIS is very efficient at separating isotopes, but it can make only a small amount in any given year. As a result, ORNL has

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Enriched Stable Isotope Prototype Plant control room.
Image credit: Carlos Jones, ORNL

Radiation, meet cancer cell

by Leo Williams
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Radiation is a double-edged sword.

While ionizing radiation—the kind that knocks electrons off atoms—can cause cancer or even death, it can also save lives. Among other uses, ionizing radiation can destroy cancer cells, giving many sufferers the hope of relief from the painful effects of cancer.

That's the goal of ORNL's nuclear medicine program. In particular, these researchers are working to exploit radioisotopes that emit alpha radiation, a type of ionizing radiation that releases a lot of energy in a very small space.

"Alpha particles penetrate only to about a 10-cell diameter or 100 micrometers—about the thickness of a human hair," explained ORNL nuclear chemist Saed Mirzadeh. "If you can target a cell—if your targeting molecule is engineered correctly, and you put these radioisotopes on as a payload—then these radioisotopes kill that cell, that specific cell, and maybe 10 cells around it."

Alpha particles are one of three types of radiation, the other two being beta particles and gamma radiation. An alpha particle consists of two protons and two neutrons, making it essentially a helium nucleus. A beta particle, on the other hand, is a high-energy electron or positron, while gamma radiation is the highest-energy form of electromagnetic radiation, putting it in the same category as microwaves, radio waves, visible light and X-rays.

ORNL has two processes for producing alpha emitters such as actinium-225, actinium-227 and lead-212. In one process, targets are bombarded at the High Flux Isotope Reactor—or, in collaboration with other national laboratories, at an accelerator—while in the other, the isotopes are separated from nuclear waste. Mirzadeh and collaborators at institutions such as the University of Tennessee College of Medicine and Memorial Sloan Kettering Cancer Center in New York City then work on ways to get the isotopes to the cancers they must destroy.

Nuclear chemist Saed Mirzadeh. Image credit: Carlos Jones, ORNL

> *"Alpha particles penetrate only to about a 10-cell diameter or 100 micrometers—about the thickness of a human hair."*
>
> — ORNL nuclear chemist **Saed Mirzadeh**

Sometimes the isotopes do the hard part—i.e., the targeting—themselves. That's the case with radium-223, which is marketed by Bayer as Xofigo. Radium-223 is a decay product of actinium-227 (currently produced at HFIR) and is used to treat prostate cancer that has spread to the bones. Because radium is chemically similar to calcium, the drug goes where calcium would go—that is, straight to bone cancer cells—and largely ignores other tissues, meaning it has few to no side effects.

Mostly, however, isotopes do not target themselves. As researchers

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designed a separate technology using gas centrifuges to enrich higher volumes of stable isotopes.

"The main thing to understand is that the electromagnetic isotope separator, the EMIS, is a high enrichment-per-pass technique, but slow, and small throughput," Hart explained.

The centrifuges—which went through a pilot production run in late 2018—also rely on the fact that different isotopes have different masses. A gas is sent past a spinning rotor, which again changes the direction of the ions based on the mass of the isotope, with heavier atoms moving to the wall and lighter ones staying closer to the center. Unlike in the EMIS, however, the result is two streams—with one made up primarily of the heaviest isotopes—instead of a separate stream for each isotope. As a result, the process involves sending the gas through a series of centrifuges—known as a cascade—to enrich the isotope incrementally.

The centrifuges are especially useful for producing large amounts of an isotope—kilograms, say, rather than grams. One highly promising isotope is xenon-129; when the isotope is inhaled by a patient, it allows an MRI to visualize the air spaces in a person's lung. In this case, the xenon would be replacing the isotope helium-3, which is in increasingly short supply.

The EMIS and centrifuges will guarantee a domestic source of stable isotopes into the future, Hart said.

"One of the drivers is to ensure that researchers in the United States have access to a domestic source of enriched stable isotopes, because foreign manufacturers may or may not be producing isotopes the researchers need," he said.

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the fluorine and reduce it to an elemental metal. Depending on the task, several more separation steps may be needed to purify the metal.

> *"I sometimes say that my day starts off accessing a room the size of an office cubicle that contains one third of a billion dollars' worth of inventory—and from that point on, my day just starts getting weird."*
>
> — ORNL materials processing researcher **Mike Zach**

In many cases, the isotope gets melted into a small bead and rolled out to the required thickness—a process that can take days. In other cases, Zach or Hickman creates a wire or cylinder by casting the melted isotope in a small mold.

The cost of the isotopes, which are housed on site, and the variety of forms they eventually take make for a unique work environment, Zach said.

"I really do have one of the most interesting jobs in the world. I sometimes say that my day starts off accessing a room the size of an office cubicle that contains one third of a billion dollars' worth of inventory—and from that point on, my day just starts getting weird."

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develop new treatments, they must overcome two major obstacles: directing the isotopes to cancer cells and keeping them from being metabolized along the way.

That second job goes to molecules known as ligands. Ligands act as baskets to hold alpha-emitting isotopes, preventing them from being hydrolyzed and excreted.

"What the ligand does is keep the metal ion intact inside this basket," Mirzadeh explained. "The body's proteins are very good at getting rid of metal ions. They just grab them and dispose of them through different mechanisms—through the liver, guts or kidneys. So we have to protect them so they don't hydrolyze."

The other job—delivering the isotope to cancer cells—goes to peptides, proteins that seek and attach to specific cells. When peptides, which have seen astonishing advances recently, are combined with the right isotope and basket molecule, they can deliver a dose of radiation selectively to cancer cells while bypassing healthy cells.

Beta and gamma radiation are also used to treat cancer, but Mirzadeh believes alpha-emitting isotopes are the future of radiation therapy. They can deliver a large amount of ionizing radiation to the targeted cells, rendering the cells unable to repair themselves. In addition, when combined with the right basket molecule and peptide, they are uniquely effective at finding and destroying the undetectable small tumors and micrometastases present in a spreading cancer.

"With all these, you don't know where the small tumors and micrometastases are," Mirzadeh explained. "If you know where the cancer cells are that you want to destroy, then of course you can knock them out, but you don't know where they are.

"Alpha emitters are about a thousand times more potent than the beta emitters. It's really clear from a scientific point of view."

Made in the USA:

Key isotopes for medical diagnostic imaging

by Dawn Levy
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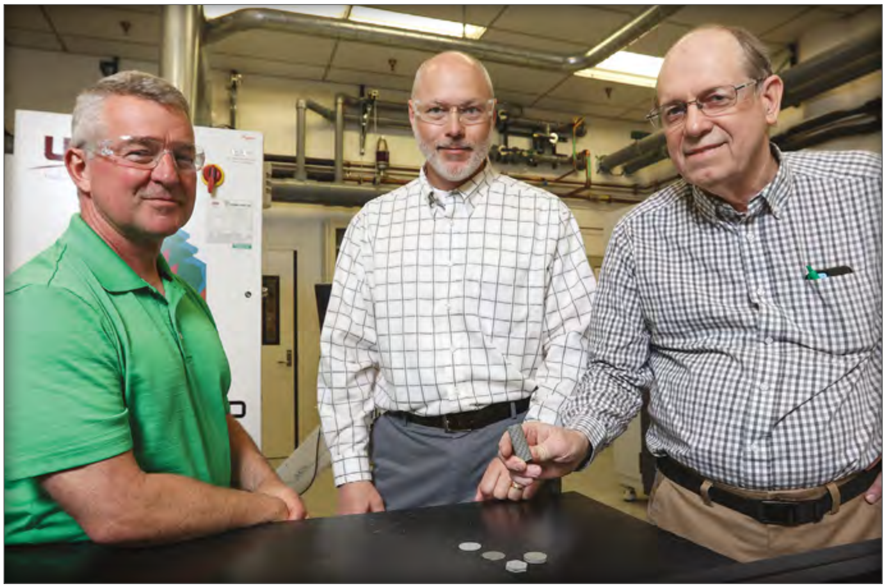
"Made in the USA." That can now be said of the radioactive isotope molybdenum-99, or Mo-99, last made in the United States in the 1980s. Its short-lived decay product, technetium-99m, is the most widely used radioisotope in medical diagnostic imaging.

In 2018, the Food and Drug Administration approved the first Mo-99 to be domestically produced without highly enriched uranium. Rather, NorthStar Medical Radioisotopes will produce Mo-99 with a neutron-capture process that employs stable molybdenum target material. Until recently, foreign vendors supplied 100 percent of the parent isotope, which was mostly produced using highly enriched uranium.

ORNL helped NorthStar make Mo-99 by a different, uranium-free method. High-energy electrons from an accelerator bombard a target enriched in Mo-100, creating intense gamma rays that knock out a neutron to make Mo-99.

"We wanted to help prepare for the commercial production of molybdenum-99 here in the United States at full-cost-recovery pricing," said Chris Bryan, who leads Mo-99 research at ORNL. The lab last year supported the efforts of several companies, including NorthStar, SHINE, Coqui and BWXT, and this year could support additional suppliers. "We were excited to assist domestic efforts that don't use highly enriched uranium."

Enriched Mo-100 is extremely expensive. Impinging electrons in the NorthStar accelerator convert less than 10 percent of the Mo-100 to Mo-99. The company must recover and recycle the remaining 90 percent.



From left, ORNL's Rick Lowden, Chris Bryan and Jim Kiggans were troubled that target discs of a material needed to produce Mo-99 using an accelerator could deform after irradiation and get stuck in their holder. The trio concluded 3D printing the entire target assembly would solve this problem. They are shown with Kiggans holding a notional target design 3D printed in natural molybdenum. Image credit: Jason Richards, ORNL

> *"Every time you handle that powder, mill it, sieve it, spray it, you lose material. The goal is to lose zero."*
> — ORNL metallurgist **Rick Lowden**

The researchers worked with other national labs to design the optimal target assembly, dissolve it to recover unconverted Mo-100, and process it into feedstock for 3D printing the next assembly.

"Every time you handle that powder, mill it, sieve it, spray it, you lose material," emphasized ORNL's Rick Lowden, a metallurgist whose team develops target materials and fabrication technologies. "The goal is to lose zero."

The ORNL team concluded the best solution was 3D printing the entire target assembly of discs in their holder.

Improving the domestic Mo-99 isotope supply chain helps more than 40,000 Americans each day get the medical images needed to map their journeys back to good health.

For more information: https://go.usa.gov/xPpV3

Titan advances cancer therapy

by Rachel Harken
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Along with surgery and chemotherapy, radiation is one of the most widely accepted forms of cancer therapy today. Until recently, most radiation therapy used photon beams in the form of X-rays to kill cancer cells, but these rays wreak havoc on healthy cells, too.

Scientists are seeking to leverage heavier particles such as protons and ions because these particles can reach deep tumors, thereby reducing radiation exposure to healthy tissues. The largest barrier to using ion beams is the size of the particle accelerators required to get these ions up to speed, but a newer type of ion acceleration that relies on lasers promises to make the hardware compact enough to fit into medical environments.

To advance this new technology, a team led by Michael Bussmann of the HZDR research laboratory in Germany used ORNL's Titan to simulate a novel laser target and validate experimental results.

The lasers used to produce proton beams typically target a foil, such as a thin piece of metal or plastic. Strong lasers can repel negatively charged electrons, pushing them out of and away from the target and leaving behind heavy ions that are accelerated to reach energies suitable to penetrate matter.

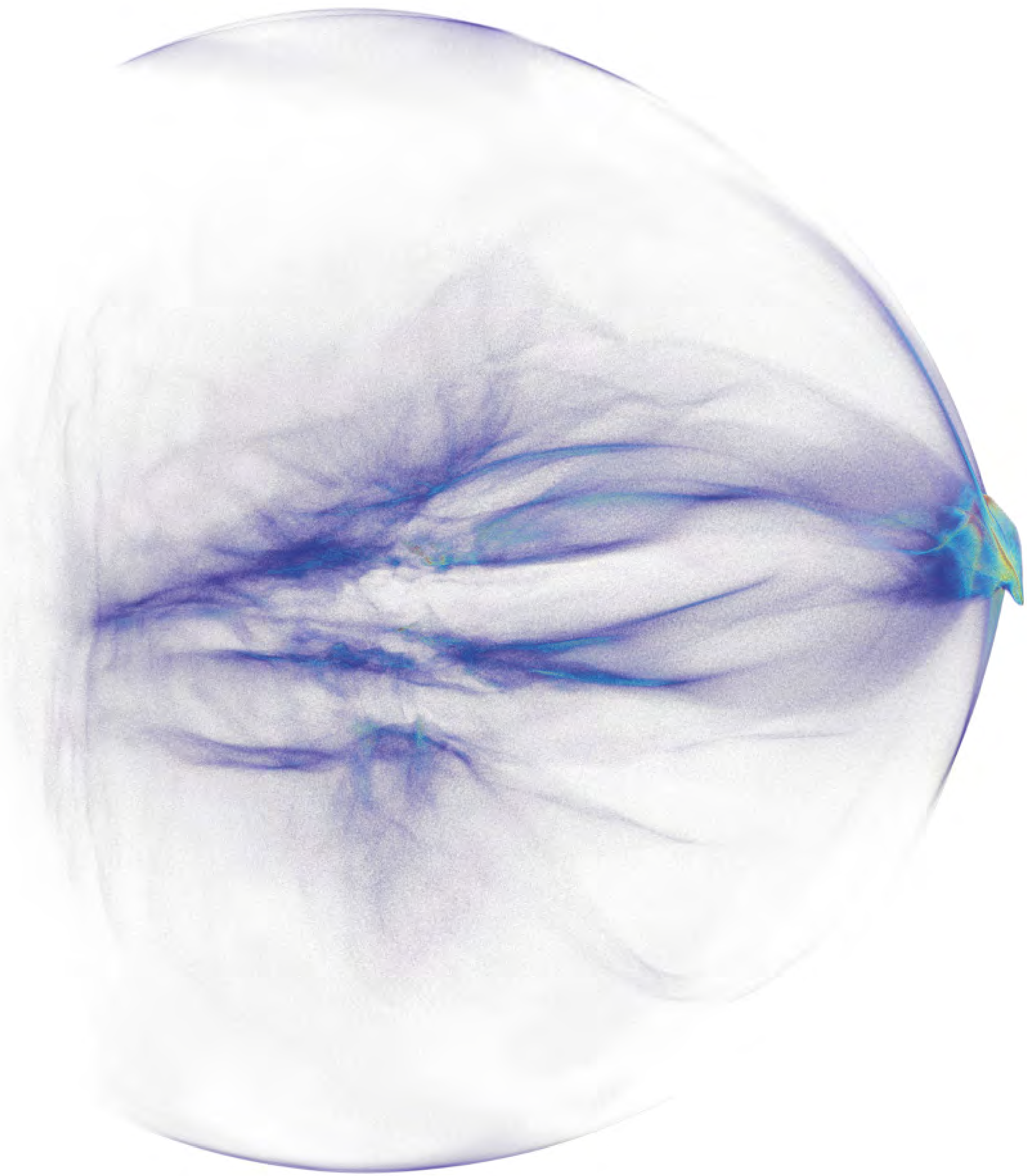
Because bulky target mounts can significantly influence the acceleration process by contributing unrelated ion signals, a team led by Joerg Schreiber of Germany's Ludwig Maximilian University and Ph.D. student Peter Hilz used the GSI Helmholtz Centre for Heavy Ion Research to test a novel plastic target that levitates freely in vacuum via a Paul trap, a configuration that uses electric fields to "trap" the target in place. With this setup, the exact number of initial protons is known beforehand, and the results of the experiment come from a "clean" proton bunch rather than from a proton bunch influenced by the target holder.

"The laser is only a couple microns wide, and the target exists at the micron scale as well," Schreiber said. "Imagine a very small ball and a slightly larger focus, and you need to overlap them in space and time."

The HZDR team simulated this experiment on Titan using a code called PIConGPU, or "particle in cell on graphics processing units," and discovered that a small shift in the strength of the laser pulse at a specific time allowed it to capitalize on the target.

"These laser pulses don't have what we call a perfect contrast," said Axel Huebl, a Ph.D. student in Bussmann's group. "They start a few picoseconds [trillionths of a second] earlier than expected, which is usually a problem. But in our simulation, since the plastic was limited to a sphere and perfectly isolated, this early start actually heated the target, exploded its size by sevenfold before the main pulse, and made it transparent to the laser. This allowed the laser to fully interact with the whole target instead of just its surface."

Image credit: Andy Sproles, ORNL



A 3D visualization of the HZDR team's final simulation of their expanded plastic target. The protons (blue) can be seen traveling along the laser axis from left to right (laser not shown). A particle bunch (red) of high-density protons can be seen on the right side. Image credit: Axel Huebl, HZDR; Peter Hilz, LMU; Michael Matheson, ORNL

The laser interacted with more of the electrons than it would have without the expansion and thus was able to put a greater amount of energy into a larger number of protons. The resulting proton beam consisted of ions with similar energies, a feature that is crucial in radiation therapy to ensure that all ions will penetrate tissue to the same depth.

"If we want to improve the laser interaction, simulations will help us get to an optimal point faster," Huebl said. "But to reach a predictive understanding, we will need to vary the experimental parameters in many more simulations."

The variability in the initial conditions is what makes simulating laser-driven ion acceleration so complex and data-intensive. Laser shape, intensity and length contribute to the physics, as do target surface texture, density and size. Individual simulations are therefore just the beginning, and the HZDR team is looking forward to gaining deeper scientific understanding from studying comprehensive ensembles of simulations.

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

The first atomic nucleus on a quantum computer

by Rachel Harken
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Quantum computing, first suggested in the 1980s by American theoretical physicist Richard Feynman, is starting to produce results.

In this new type of computing, the bits that carry information are replaced by qubits (pronounced CUE-bits)—particles such as electrons and photons that carry the information in their quantum states.

In 2010, a team at the University of Queensland led by B. P. Lanyon simulated a hydrogen molecule, H_2, on a quantum system for the first time. Then, last fall, research scientists at IBM performed the first quantum calculations of molecules beyond hydrogen and helium.

Now a team at ORNL has gone deeper, successfully simulating an atom's nucleus using a quantum computer by calculating the nucleus' binding energy, the minimum energy needed to disassemble it into its subatomic particles.

In October 2017, the ORNL team started developing codes to perform simulations on the IBM QX5 and the Rigetti 19Q quantum computers. Using freely available pyQuil software, a library designed

This illustration shows a deuteron, the bound state of a proton (red) and a neutron (blue).
Image credit: Andy Sproles, ORNL

for producing programs in the quantum instruction language, the researchers wrote a code that was sent first to a simulator and then to the cloud-based IBM and Rigetti systems.

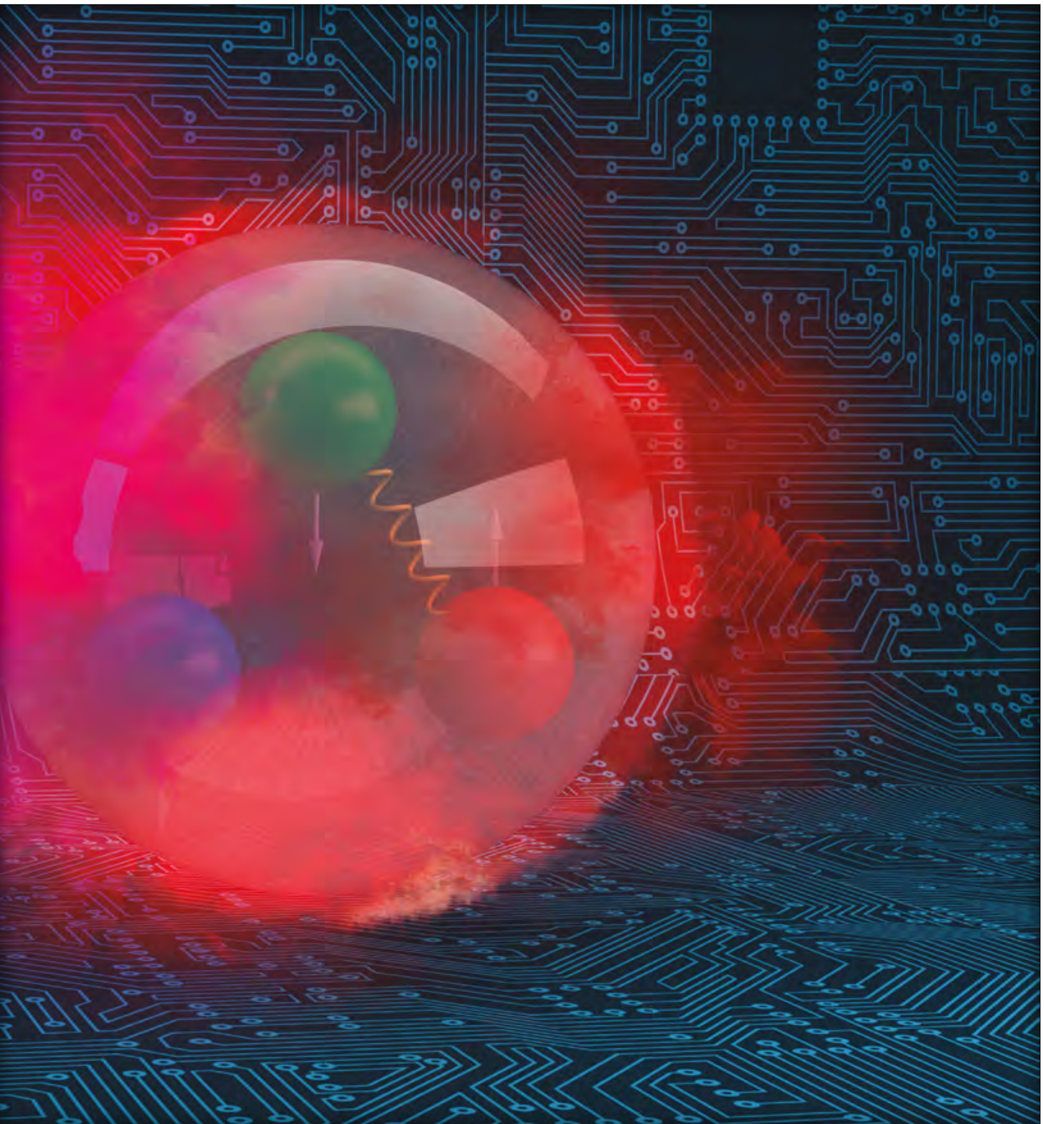
algorithms for the project as part of the Nuclear Theory Group at ORNL.

Whereas a bit must be in only one of two states, a qubit's power rests in its ability to be in a combination of two states—a principle known as quantum superposition.

> *"In classical computing, you write in bits of zero and one. But with a qubit, you can have zero, one, and any possible combination of zero and one, so you gain a vast set of possibilities to store data."*
> — ORNL physicist **Thomas Papenbrock**

The team performed the simulations under DOE's Quantum Testbed Pathfinder project, an effort to verify and validate scientific applications on different quantum hardware types. Gustav Jansen, a computational scientist in the Oak Ridge Leadership Computing Facility's Scientific Computing Group, played a role in testing

"In classical computing, you write in bits of zero and one," said Thomas Papenbrock, a theoretical nuclear physicist at the University of Tennessee and ORNL who co-led the project with ORNL quantum information specialist Pavel Lougovski. "But with a qubit, you can have zero, one, and any possible combination of zero and one, so you gain a vast set of possibilities to store data."



The team performed more than 700,000 quantum measurements of the energy of a simulated deuteron, the nuclear bound state of a proton and a neutron. In quantum computers, measurements are variable because they rely on qubits that begin in a state of superposition, affecting the outcome of each run. Performing such a large number of measurements allowed the scientists to narrow down the solution and, ultimately, extract the deuteron's binding energy. The deuteron is the simplest composite atomic nucleus, making it an ideal candidate for the project.

"Qubits are generic versions of quantum two-state systems. They have no properties of a neutron or a proton to start with," Lougovski said. "We can map these properties to qubits and then use them to simulate specific phenomena—in this case, binding energy."

At the completion of the project, the team's results on two and three qubits were within 2 and 3 percent, respectively, of the correct answer on a classical computer, and the quantum computation became the first in the nuclear physics community.

The proof-of-principle simulation paves the way for computing much heavier nuclei with many more protons and neutrons on quantum systems. Quantum computers have potential applications in cryptography, artificial intelligence, and weather forecasting because each additional qubit becomes entangled—or tied inextricably—to the others, exponentially increasing the number of possible outcomes for the measured state at the end.

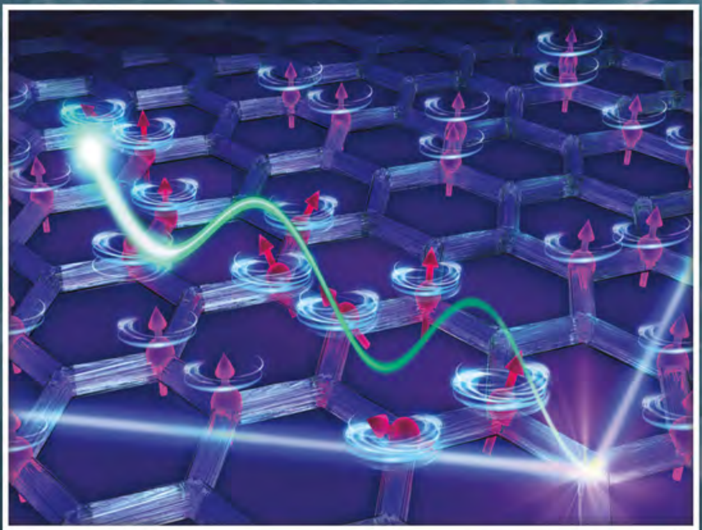
Papenbrock said the team hopes that improved hardware will eventually enable scientists to solve problems that cannot be solved on traditional supercomputers alone. In the future, quantum computations of complex nuclei could unravel important details about the properties of matter, the formation of heavy elements, and the origins of the universe.

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

The Art of Science

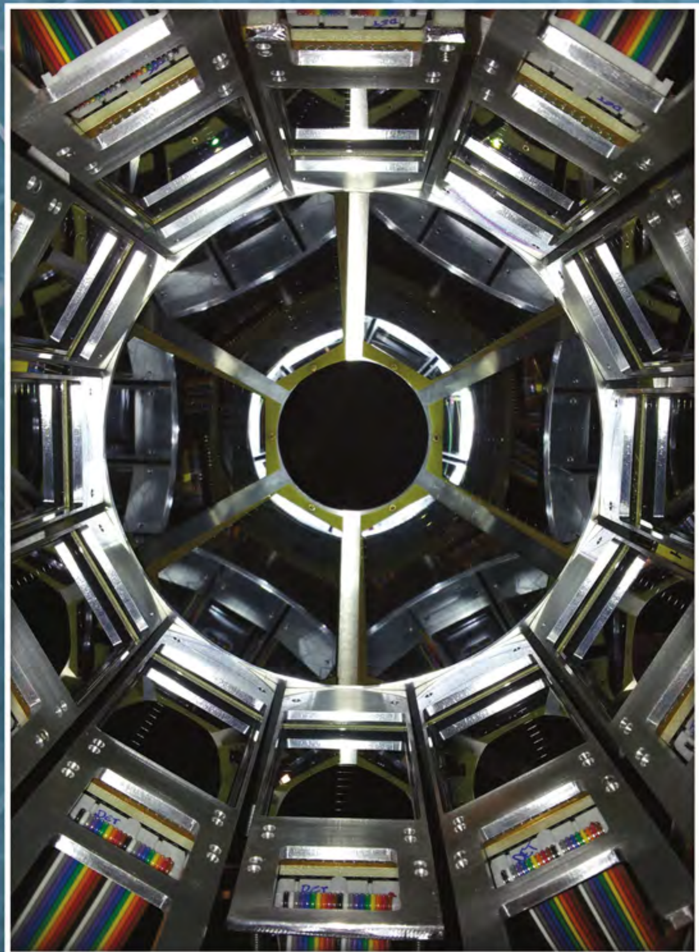
Ninety images were submitted recently to ORNL's first Art of Science Competition, which aims to share scientific discovery and knowledge through visually compelling images. You can see a sampling here, with more images available at bit.ly/2C2MOGW.

Photons of Light, submitted by Peyton Ticknor, won "Peoples Choice."
Image credit: Jason Richards and Brett Hopwood, ORNL

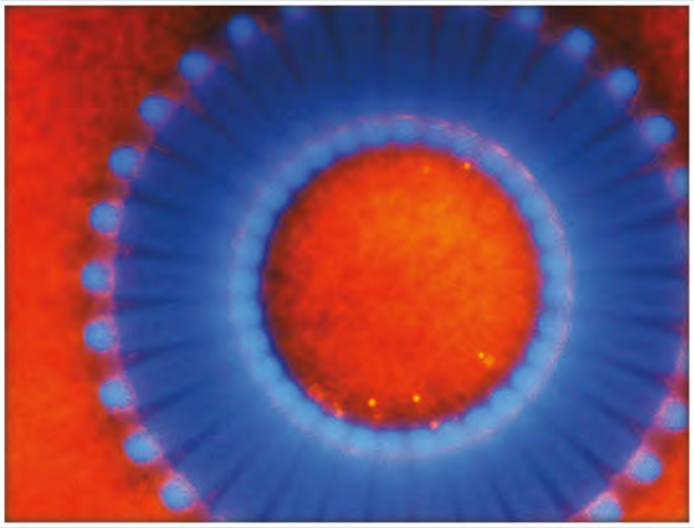


Majoranas on Honeycomb won "Directors Choice."
Image credit: Jill Hemman, ORNL

Micro Tumbleweeds.
Image credit: Bernadeta Srijanto and Dale Hensley, ORNL

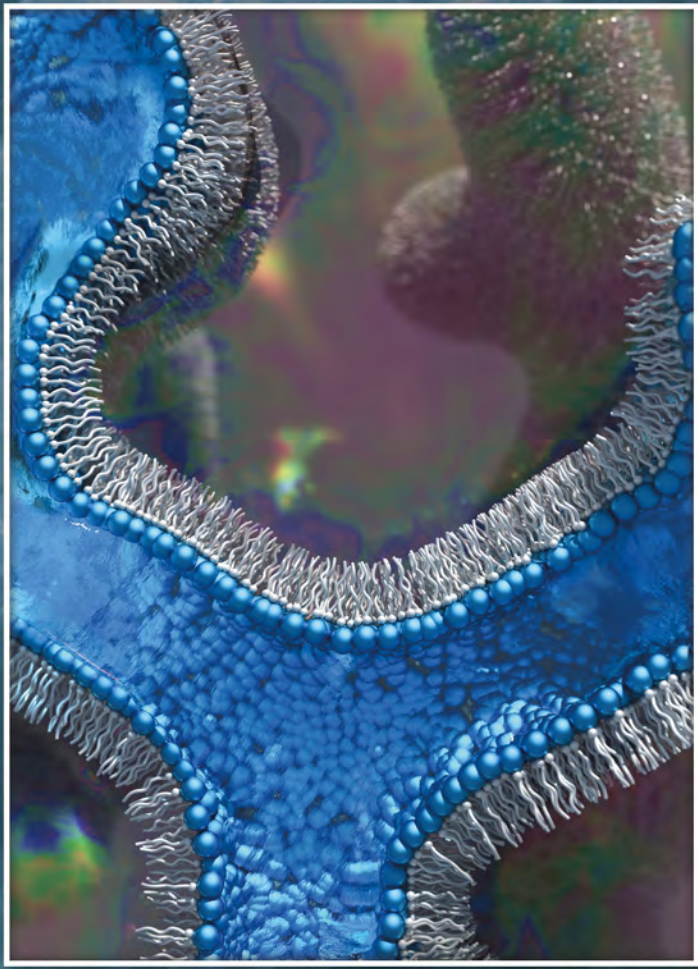


Beam's Eye View.
Image credit: Steven Pain, ORNL

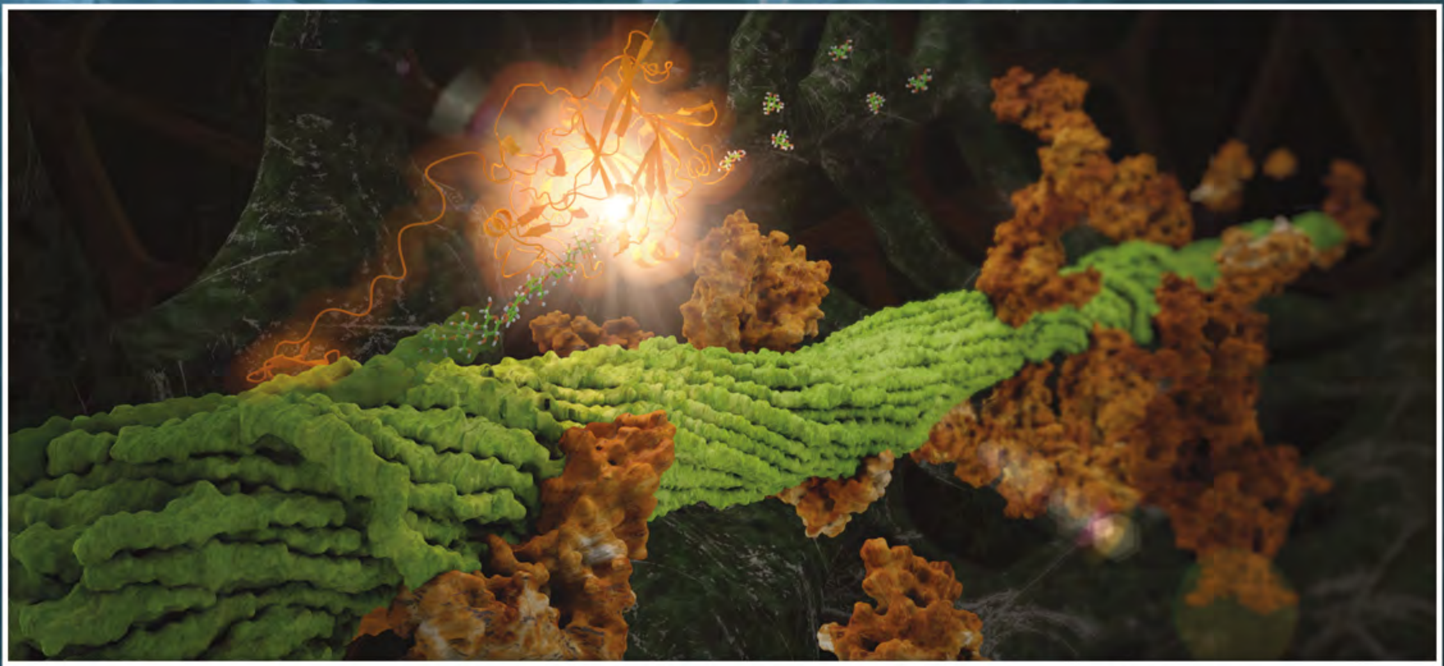


The Eye of Sauron.
Image credit: Bernadeta Srijanto, ORNL

Sample Environment.
Image credit: Genevieve Martin, ORNL



Bijels. Image credit: Jill Hemman in support of research by Caili Huang, Weiyu Wang and Kunlun Hong



Biomass for Bioenergy.
Image credit: Loukas Petridis, ORNL

Researchers take temperatures

at the nanoscale

by Dawn Levy
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A scientific team led by ORNL has found a new way to take the local temperature of a material from an area about a billionth of a meter wide, or approximately 100,000 times thinner than a human hair.

This discovery promises to improve the understanding of useful, yet unusual, physical and chemical behaviors that arise in materials and structures at the nanoscale. The ability to take nanoscale temperatures could help advance microelectronic devices, semiconducting materials and other technologies, whose development depends on mapping atomic-scale vibrations due to heat.

The study used a technique called electron energy gain spectroscopy in a newly purchased, specialized instrument that produces images with both high spatial resolution and great spectral detail. The 13-foot-tall instrument, made by Nion Co., is named HERMES, short for high energy resolution monochromated electron energy-loss spectroscopy-scanning transmission electron microscope.

Atoms are always shaking. The higher the temperature, the more the atoms shake. Here, the scientists used the new HERMES instrument to measure the temperature of semiconducting hexagonal boron nitride by directly observing the atomic vibrations that correspond to heat in the material.

"What is most important about this 'thermometer' that we have developed is that temperature calibration is not needed," said physicist Juan Carlos Idrobo of ORNL's Center for Nanophase Materials Sciences.

These two features are depicted as peaks, which are used to calculate a ratio between energy gain and energy loss. "From this we get a temperature," Lupini explained. "We don't need to know anything about the material beforehand to measure temperature."

In 1966, H. Boersch, J. Geiger and W. Stickel published a demonstration of electron energy gain spectroscopy at a larger length scale and pointed out that the measurement should depend upon the temperature of the sample. Based on that suggestion, the ORNL team hypothesized that it should be possible to measure a nanomaterial's temperature using an electron microscope with an electron beam that is "monochromated," or filtered to select energies within a narrow range.

> *"The new HERMES lets us look at very tiny energy losses and even very small amounts of energy gain by the sample, which are even harder to observe because they are less likely to happen."*
>
> — ORNL physicist **Juan Carlos Idrobo**

Other thermometers require prior calibration. To make temperature graduation marks on a mercury thermometer, for example, the manufacturer needs to know how much mercury expands as the temperature rises.

"ORNL's HERMES instead gives a direct measurement of temperature at the nanoscale," said Andrew Lupini of ORNL's Materials Science and Technology Division. The experimenter needs only to know the energy and intensity of an atomic vibration in a material—both of which are measured during the experiment.

To perform experiments using electron-energy-gain-and-loss spectroscopy, scientists place a sample material in the electron microscope. The microscope's electron beam goes through the sample, with most electrons barely interacting with it. In electron-energy-loss spectroscopy, the beam loses energy as it passes through the sample, whereas in energy-gain spectroscopy, the electrons gain energy from interacting with the sample.

"The new HERMES lets us look at very tiny energy losses and even very small amounts of energy gain by the sample, which are even harder to observe because they are less likely to happen," Idrobo said.

"The key to our experiment is that statistical physical principles tell us that it is more likely to observe energy gain when the sample is heated. That is precisely what allowed us to measure the temperature of the boron nitride."

Nanoscale resolution makes it possible to characterize the local temperature during phase transitions in materials—an impossibility with techniques that do not have the spatial resolution of HERMES spectroscopy.

For more information: go.usa.gov/xP9rP

Andrew Lupini, left, and Juan Carlos Idrobo use ORNL's new monochromated, aberration-corrected scanning transmission electron microscope to take the temperatures of materials at the nanoscale. Image credit: Jason Richards, ORNL

Power to the people:

Solutions for a better Puerto Rico grid

by Stephanie Seay
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As Hurricane Maria swirled out to sea after plowing a destructive path across Puerto Rico in September 2017, initial reports were clear: The island's power grid lay in near ruin.

DOE and its national laboratories immediately got busy, working not only to offer solutions for rebuilding the island's electricity network but also to make it resilient to future disruption.

At ORNL, researchers stepped in to develop models for better grid protection, analyze options for new generation sources, and deploy sensors to monitor and evaluate the grid and inform decisions by the island's utility, the Puerto Rico Electric Power Authority.

One key development has been a planning model that places and optimizes systems called "protective relays," which control circuit breakers and can isolate areas where power lines may be down, preventing outages from cascading system-wide. ORNL's Dynamic Protection-Planning Model can be used to predict the behavior of the electrical system in the event of severe weather.

The tool can, for instance, take the projected path of a hurricane and analyze its impact on transmission equipment, said Nils Stenvig of ORNL's Power and Energy Systems Group. Such information can be crucial for planning and recovery.

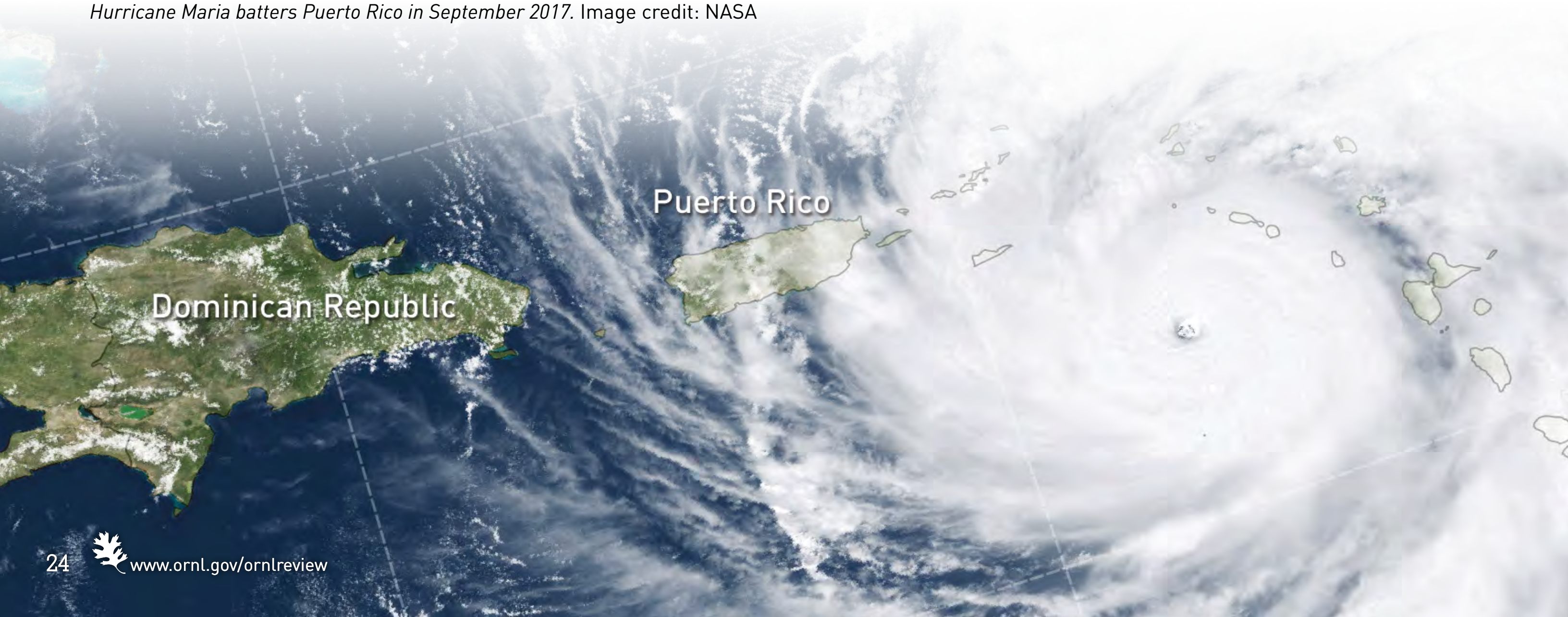
The model could support tasks such as predictive islanding: isolating portions of the grid expected to be hit the hardest to keep as much of the system running as possible during a storm, Stenvig noted.

Travis Smith, an ORNL protection system engineer who has worked for major utilities, had already developed advanced modeling tools for DOE that take into account protective relays. He expanded those simulations for the Puerto Rico project.

"Protection engineers know how to calibrate relays individually, but this tool gives them a way to analyze and coordinate the entire system and make improvements," Smith said. "This is a real roadmap utilities can use to modernize their system."

Another tool being developed for Puerto Rico analyzes locations where new power generation can be sited and integrated into the grid without costly transmission system upgrades. "Sometimes those transmission system upgrades can end up costing more than the new generation itself," Stenvig said.

Hurricane Maria batters Puerto Rico in September 2017. Image credit: NASA



From left, Nils Stenvig, Isabelle Snyder and Travis Smith of ORNL's Power and Energy Systems Group stand in front of a digital simulator, which allows them to simulate grid equipment. Snyder is holding a GridEye sensor. Image credit: Carlos Jones, ORNL

ORNL's computational scientists are also evaluating locations on the island where equipment such as spare generators and transformers could be strategically placed for easy, secure access after a natural disaster.

To help visualize the grid in Puerto Rico and validate modeling, ORNL researchers are in the process of deploying 20 GridEye sensors that constantly monitor and report on the island's grid.

GridEye sensors, developed by University of Tennessee/ORNL Governor's Chair Yilu Liu, have already been deployed at hundreds of locations across the continental United States to provide wide-area situational awareness of the grid. The sensors plug into standard household outlets and record data on electrical disturbances using a patented triangulation algorithm.

The sensors are located inside utility substations, universities and commercial buildings in Puerto Rico. They are connected to the internet and synchronized with one another via a global positioning system to provide voltage, frequency and other measurements and to ensure the accuracy of researchers' models.

In another project, ORNL is working to promote the island's economic vitality by analyzing potential investments in microgrids. The microgrids would be made up of power generated around the island combined with energy storage. Microgrids have become increasingly popular to diversify a utility's generation mix. ORNL researchers are working with collaborators at Sandia National Laboratories to provide technical analysis of proposed microgrid projects.

"Microgrids would make a real impact on businesses across the island," Stenvig said. "They could potentially supply power to surrounding neighborhoods as well."

ORNL researchers are also conceiving a more flexible system of utility poles that could, for instance, bend rather than break in high winds or could be safely collapsed ahead of a storm and then unfolded afterward. The lab's expertise and capabilities in additive manufacturing could be leveraged to more quickly design and produce such infrastructure.

The research "fits into everything we do here at ORNL in terms of materials science, sensing, electronics, simulation, high-performance computing, and cyber-physical security," Smith said.

Vacuum insulation panels open the door to self-healing buildings

Jennifer Burke
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A building's exterior endures wear and tear from natural elements over time. Wind, rain, snow and even harsh sunlight can do costly damage. But what if a building could heal itself from cuts, tears and punctures, saving time and cost?

It may sound better suited for science fiction, but ORNL's Building Envelope & Urban Systems Research Group may have found the answer to self-healing buildings by creating a novel multilayered barrier film with self-healing properties for vacuum insulation panels—or VIPs.

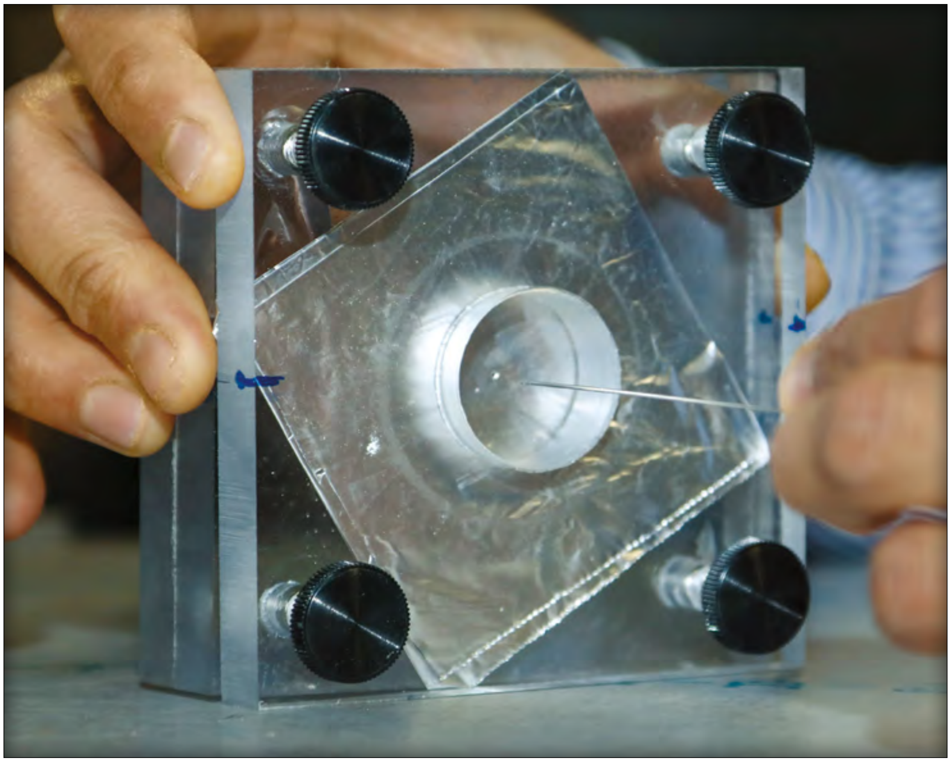
VIPs consist of a silica, aerogel or glass fiber core with the air removed that is encapsulated within an impermeable-barrier envelope. Because of their internal vacuum, VIPs are five to 10 times better at reducing unintended heat losses and gains through building walls and roofs than conventional materials such as polystyrene and fiberglass insulation.

Although VIPs have proved to be more efficient, they've yet to be fully embraced by America's building industry. Kaushik Biswas, a mechanical engineer and lead researcher on the self-healing project at ORNL, said a major reason for slow adoption comes down to durability.

"VIPs are more widely used in Europe," Biswas said. "However, there are concerns about their durability, and that has partly prevented them from being used as building insulation in the U.S. A common question from industry is, 'What if someone puts a nail through a VIP?' My answer is, 'But what if we can develop a type of panel that can heal from punctures?' It removes one of the major barriers to adoption of VIPs in buildings."

Biswas has spent the better part of the past year working with ORNL Chemical Sciences Division researchers Tomonori Saito and Pengfei Cao to optimize the self-healing chemistry, demonstrating proof of concept through laboratory experiments.

The team conducted experiments to see if small-scale samples could self-heal after penetration—and they did. "We performed a limited number of experiments on 2-by-2-inch samples, and they were successful," Biswas said. "The next



Vacuum insulation panel. Image credit: Genevieve Martin, ORNL

ORNL researcher Kaushik Biswas demonstrates how a self-healing barrier in a vacuum insulation panel can recover from a puncture.
Image credit: Genevieve Martin, ORNL

step is to determine how we scale up to films that can be used as the barrier envelopes of VIPs."

The team has started working on scaled-up self-healing films for VIPs.

"We had some challenges coming up with the correct chemical formulation, but we think we have identified an appropriate combination," Biswas said. "Self-healing barriers are a potentially game-changing technology because they can seal cuts and punctures and maintain the internal vacuum in VIPs, overcoming durability concerns."

The work is a high priority for DOE's Building Technologies Office, too, because some 40 percent of the nation's energy is consumed in residential and commercial buildings.

Combining materials research with heat transfer principles has been a primary focus of Biswas' work at ORNL. He's part of a research team with industry partners NanoPore and Firestone Building Products Company that developed a 2-inch-thick composite foam–VIP insulation board that can achieve thermal resistance of R25, more than twice that of typical insulation used in buildings.

The composite boards contain a lower-cost VIP called modified atmosphere insulation, which was developed by NanoPore. Biswas is also part of a team of researchers investigating alternative thermal management techniques for buildings, new kinds of vacuum insulation and energy storage technologies.

"VIP-based composites are technically viable options for buildings, providing higher performance than current insulations," Biswas said. "We continue to develop new ways to improve the energy performance of building envelopes, including vacuum insulation."

Investigating Arctic ecosystems: A conversation with Stan Wullschleger

by Kim Askey
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For the past six years, some 140 scientists from five institutions have traveled to the Arctic Circle and beyond to gather field data as part of the DOE-sponsored Next-Generation Ecosystem Experiments Arctic or NGEE Arctic project. The research teams integrate this data into Earth system models to improve predictions of environmental change.

Stan Wullschleger, director of ORNL's Environmental Sciences Division, leads the NGEE Arctic project, orchestrating a flow of scientific teams journeying to Utqiagvik and Nome, Alaska, to gather measurements. The 10-year project draws on expertise in diverse disciplines such as hydrology and biogeochemistry from researchers at Oak Ridge, Los Alamos, Brookhaven and Lawrence Berkeley national laboratories and the University of Alaska–Fairbanks.

We talked with Wullschleger about the discoveries and challenges of the NGEE Arctic project. This is an edited transcript.

Why go to the Arctic Circle?

The Arctic is an important region for investigating the interactions between land and atmospheric processes and how these feedbacks affect climate. The Arctic is warming at a rate twice that of the global average, and the consequences of this warming will shape the ecology of this region in many ways. Changes in environmental processes like carbon cycling and

A researcher measures snow depth at the Kougarok field site. Image credit: Bob Bolton, University of Alaska

The NGEE Arctic team collects snow samples from the arctic tundra. Image credit: Stan Wullschleger, ORNL

NGEE Arctic scientists prepare to head out to field sites in Nome, Alaska. Image credit: Stan Wullschleger, ORNL

shrub migration are being accelerated in the Arctic more than anywhere else on the planet. Our goal is to measure it, translate data into equations, and incorporate those into computer models.

Arctic soils also hold a significant amount of stored carbon. We are interested in the sensitivity of these very ice-rich ecosystems to a warming climate. The freezing point of water becomes a tipping point for many physical, chemical and biological processes in these cold regions. As the soil thaws, microbes break down organic matter that has been frozen in permafrost for hundreds, if not thousands, of years and release carbon dioxide and methane into the atmosphere.

What is the advantage to having field sites in both Utqiagvik and Nome, Alaska?

We started in Utqiagvik, on the north slope of the Alaskan coast where soil temperatures year-round are minus 20°F or colder. Then we added Nome, which is located on the west coast just within the Arctic Circle and has a warmer climate. Soils and permafrost there are right at the freezing point, which makes for a much more dynamic landscape. These sites give us two ends of a continuum of very cold to warm permafrost that we can compare and contrast, studying environmental processes along temperature and latitudinal gradients. That gives us a lot of power in trying to understand not only current ecosystem processes, but also what ecosystems might look like in the future.

What are the toughest challenges you face?

Early in the project, we had a steep learning curve. Most of us had never worked in the Arctic before, and our partners at the University of Alaska–Fairbanks were instrumental in helping us establish protocols for working safely and productively in these cold, remote landscapes. They also helped us establish key relationships with the native corporations that own the lands we study.

You have to be really prepared and develop your work plans ahead of time. You have to make sure that when you hop out of your vehicle, or off the snow machine, or off the helicopter into a hoard of mosquitos or temperatures that can dip below minus 20°F, you have everything you need for that day, because you're not going to get a second chance to run to the store to grab something you forgot.

Did anything in this project surprise you?

The complexity of the ecosystem surprised me. We knew going in that we were going to study certain processes, such as vegetation dynamics and the microbial production of carbon dioxide and methane. But as it turns out, all of those processes are coupled and interconnected; and because of that, we've changed how we study the system. We had to rethink our experimental approach, how we collect data, how we interact as a team, and then how we bring all of that data together for models. It's been a great experience for all the members of our team—students to senior scientists—and this integrated approach enriches the scientific outcomes.

ITER's 'burning plasma':

One giant step toward fusion energy

by Jim Pearce
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A December 2018 report by the National Academies ushered in the new year by re-affirming strong support for U.S. participation in the ITER Project and "increased attention to engineering and technology-based development."

The doughnut-shaped ITER will, for the first time on Earth, create a burning (self-heating) plasma and contain it with a magnetic field. The plasma itself will be heated and sustained primarily by its own fusion reactions—literally the same energy source that powers the sun and the stars.

So, what does the ITER experiment provide that makes this leap forward possible? ITER will be the first fusion device to produce net thermal energy, meaning the total thermal power produced by a fusion plasma pulse is greater than the thermal power injected to heat the plasma. It is expected to generate 500 megawatts of thermal power for every 50 megawatts of thermal power injected to heat the plasma.

The experiment will also be the first to maintain a fusion reaction for minutes at a time, rather than seconds. And finally, ITER will be a proving ground for many systems, materials and technologies needed to develop commercial-scale fusion reactors. When ITER succeeds in producing a burning (self-heating) plasma, commercial-scale fusion energy will move firmly into the realm of the possible.

Why fusion?

The prospect of harnessing fusion is compelling for a number of reasons. First, the primary fuel, deuterium, can be extracted from ordinary seawater. The other main ingredient, tritium, can be produced from lithium, which is also widely available. Moreover, fusion reactors will not produce carbon emissions or greenhouse gases and will recycle most of their fuel. Finally, the low-level, short-lived radioactive waste generated by fusion reactions is mainly in the form of activated structures (reactor components that become radioactive); these require only a human lifetime to decay to safe levels.

When asked to describe one idea that would transform our society, the late Stephen Hawking said, "I would like to see the development of fusion power that gives an unlimited supply of clean energy and a switch to electric cars. Nuclear fusion would become a practical power source that would provide us with an inexhaustible supply of energy without pollution or global warming."

Construction is advancing steadily on the ITER tokamak complex and supporting facilities in France, while components are in fabrication around the globe. Image credit: ITER Organization

When ITER reaches "first plasma" in 2025, the international ITER project will begin to address Hawking's vision of inexhaustible energy, but it will be more than just the culmination of decades of fusion science and engineering. It will embody the confluence of technological advances from across the scientific spectrum that are necessary before scientists and engineers can tackle the challenge of constructing the first fusion power station.

Broader impact

As in previous "big science" projects such as the International Space Station or the Large Hadron Collider, knowledge gained through the ITER experiment will expand not only the boundaries of its own field of plasma physics but those of science in general. Because of the project's sheer scale and complexity, ITER has already led to advances in an array of industrial technologies, including superconducting magnets, vacuum technologies, cryogenics, and robotic systems for handling materials.

Global game changer

Once ITER is completed, experiments will begin to provide answers to questions that are critical to the construction of a fusion power station, including:

- How does a reactor-scale burning plasma behave? What are the implications of producing fusion power at a mass scale for electricity?
- Does burning plasma behave differently when it is being sustained by its own fusion reactions rather than heated by external sources?
- How does a burning plasma affect the performance of components and systems needed for a fusion reactor?

Based on knowledge and experience acquired through research conducted on ITER and other fusion research devices, most experts expect commercial fusion power generation to become a reality in the mid- to late 21st century.

Energy Secretary Rick Perry recently characterized the ITER experiment and fusion energy as global game changers.

"If we can deliver fusion energy to the world," he said, "we've changed the world forever."

Unveiling quantum materials with neutrons

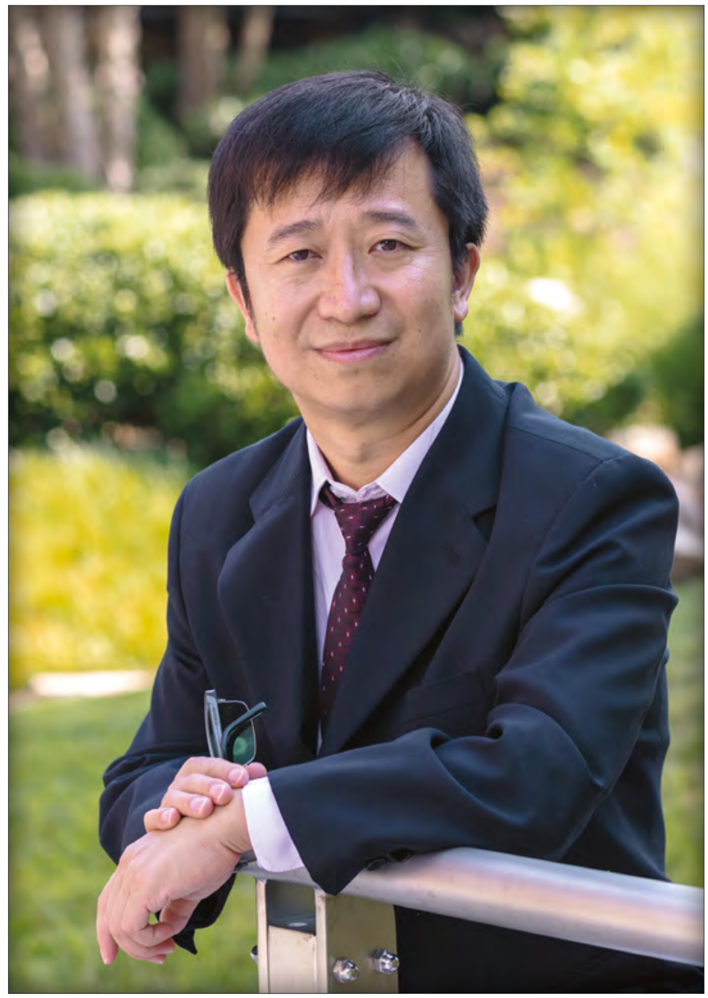
A conversation with scientist Huibo Cao

The next great materials discovery may well come from the exotic interactions of electrons at a scale a million times smaller than a human hair. This is the scale of quantum physics, and it's where ORNL's Huibo Cao focuses his efforts.

Cao grew up in the Shanxi province of northern China, in a small village called Shuiquan. After earning a bachelor's degree in physics from Shanxi University and a Ph.D. in condensed matter physics from the Institute of Physics, Chinese Academy of Sciences, in Beijing, he took a postdoctoral position at the Laboratoire Léon Brillouin at the Alternative Energies and Atomic Energy Commission–Saclay in France.

He came to ORNL in 2009, working through Oak Ridge Associated Universities, and joined the lab's staff in 2013 as an instrument scientist at the High Flux Isotope Reactor.

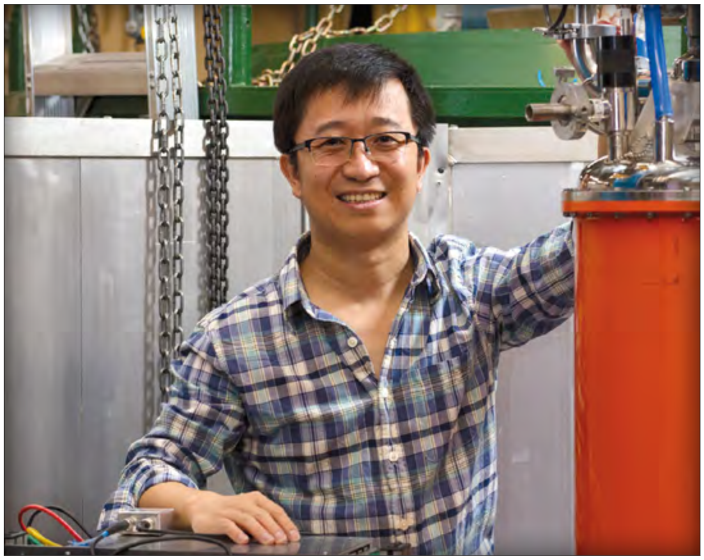
Cao won a 2018 Early Career Research Program award from DOE's Office of Science for his proposal "Local Site Magnetic Susceptibility for Quantum Materials by Polarized Neutron Diffraction." We talked with him about the project and about what drew him to a career in science. This is an edited transcript.



1. What are quantum materials?

Quantum materials are materials that exhibit properties or phenomena that cannot be understood by classical or semi-classical theory. In condensed matter physics, quantum materials can be defined as solids with exotic electron properties, unconventional spin orders, abnormal phonon behaviors, or other phenomena resulting from the subtle balance of competing interactions among quantum properties such as spin, orbital, charge and lattice degrees of freedom.

Quantum materials include superconductors, which exhibit no electrical resistance; multiferroics, which exhibit both magnetic and electric polarizations; spin ices, whose magnetic moments show disorder like the disorder of protons in regular ice; spin liquids, in which electron spins are random; and a variety of other phenomena you can only find at the nanoscale. Understanding these systems requires us to detect the couplings of different variables and their subtle balance at atomic and subatomic scales. Neutrons are small quantum magnets and provide an ideal tool for detecting magnetic order and coupling.



2. How will you study quantum materials with this project?

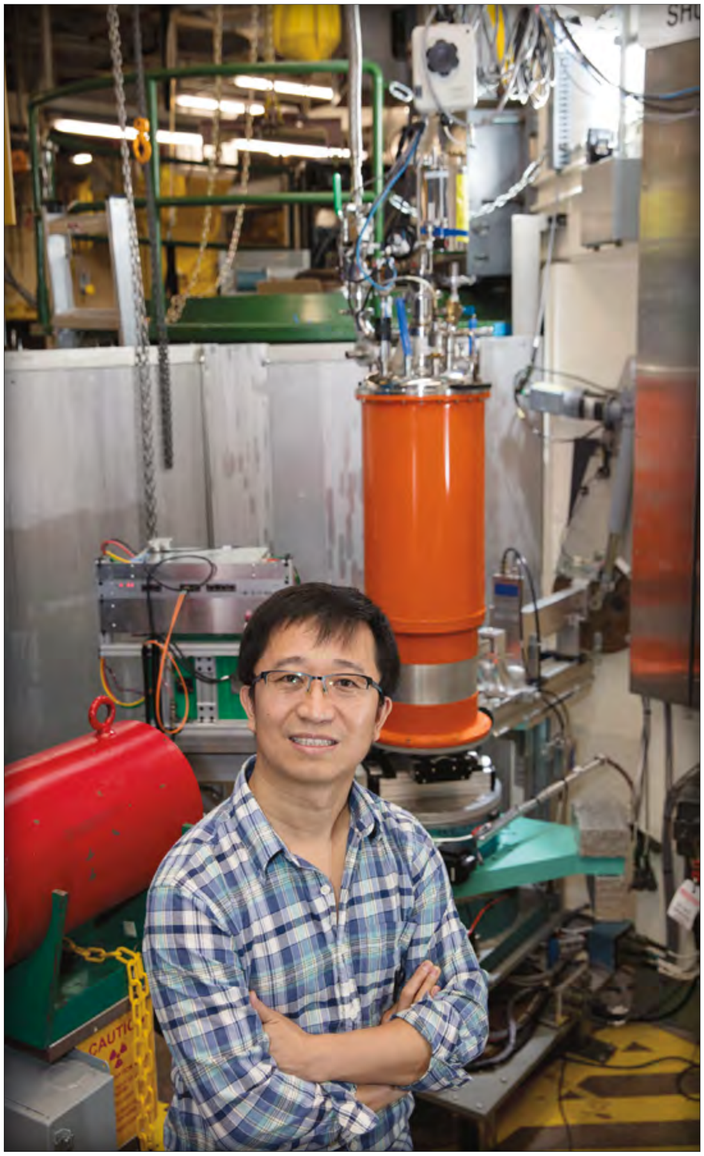
This project uses polarized neutrons—in which spins are polarized in the same direction—to detect magnetic susceptibilities to applied fields and visualize magnetic density distributions. They can also determine the coupling of spin, orbital and lattice degrees of freedom.

Polarized neutrons are more sensitive to spin components than non-polarized neutrons and provide a way to detect a field-induced spin response at each atomic site. This reveals a site's magnetic strength from neighboring sites and the local environment.

In addition, by reconstructing maps of spin density in the whole lattice, we can directly show magnetic interaction paths and possible orbital order and hybridization—that is, the mixing of orbitals.

With this information, we expect to build a complete Hamiltonian description of a quantum magnetic system describing the total energy in the system.

If we succeed, we will be able to measure small crystals of quantum materials, as well as small crystals under high pressure, thereby speeding the study of quantum materials. Success will also enable us to study and calibrate a system with the same sample, avoiding the confusion of quantum behaviors from impurity and chemical disorder.



3. How will a new understanding of quantum materials be helpful?

Understanding the subtle balance of interactions among all the degrees of freedom in a given quantum candidate material can guide the design of, or search for, new, better or true quantum materials, and can help us explore more properties originating from quantum mechanics.

4. What attracted you to science?

I was attracted to science by the beauty of physics, and I was curious about the laws that governed the physical world. In high school, I was impressed by Newton's laws of motion. In college, Einstein and Schrödinger taught me about uncertainty. Now I am excited to observe the beauty of magnetism by neutrons and curious about the laws governing exotic states and fascinating phenomena.

Flash of light:

A conversation with spectroscopist Ben Doughty

What does a high school grad do when his family threatens to make him pay rent? For ORNL spectroscopist Ben Doughty, the answer was, go to college.

Doughty avoided the threatened stay-at-home tax by enrolling at the University of Florida, where he discovered a talent for chemistry. He followed up his undergrad career with a Ph.D. from the University of California at Berkeley, a postdoctoral position at Columbia University and a Wigner fellowship at ORNL.

Doughty won a 2018 Early Career Research Program award from DOE's Office of Science for his proposal "Chemical Organization, Structure and Dynamics at Complex Liquid-Liquid Interfaces: Mechanistic Insight into Selective Solvent Extraction and Self-Assembly." We talked with him about the project and about what drew him to a career in science. This is an edited transcript.

1. Why is the interface between liquids important?

There is a lot of interesting chemistry that happens at that interface. What we are interested in is really understanding how molecules or atoms or individual ions are transported across the interface. This has applications in nuclear waste cleanup and separating materials for purification processes. There are lots of technological reasons why you would want to separate two things from each other, and a liquid-liquid interface happens to be a very good way to do that. The molecular machinery does a very efficient job, but we don't quite understand how it works.

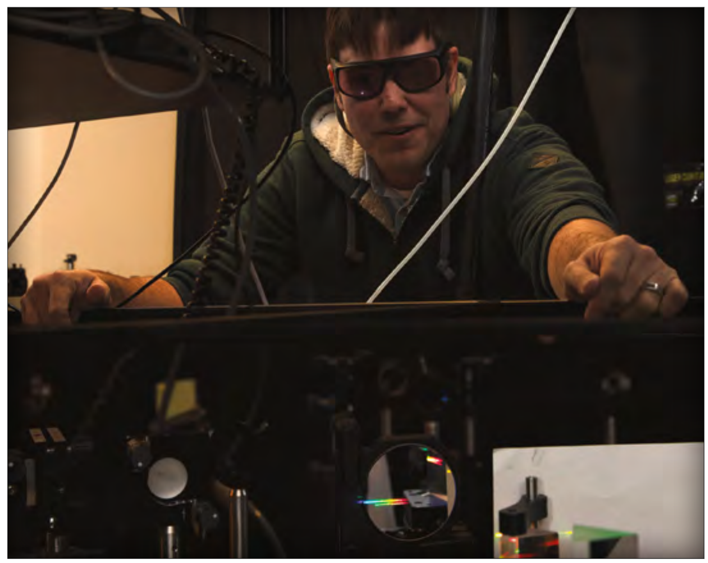
2. How will you go about understanding the liquid-liquid interface?

I specialize in a field of laser spectroscopy called nonlinear optics using techniques called sum-frequency generation and second harmonic generation.

We take two very intense, very short laser pulses that last 50 femtoseconds—that's 50 millionths of a billionth of a second, so you have an immense amount of energy crammed into a very short time window. When you overlap two pulses at a sample, you can generate new colors, where you add and subtract the individual laser frequencies inside of those pulses. And whenever there's a molecule at an interface that absorbs light in one of those laser packets, you get an enhanced signal. So what you end up getting is a spectrum that now reports on just the interface, just the surface.

The tools that we developed in the lab are really designed to target complicated interfaces, and a liquid-liquid interface is one of the more complicated things you can look at. It sounds simple—just oil and water—but there are a lot of subtleties that are very poorly understood.

We are also bringing in neutron scattering measurements to give complementary information. With the nonlinear techniques that we use, we can get information about orientation, hydrogen bonding and chemical speciation in the molecular plane. With neutron scattering, you get information about how molecules are ordered out of the plane, above and below.



3. What will we be able to do with a better understanding of the liquid-liquid interface?

Right now our understanding of an interface for separations purposes is based on a thermodynamic perspective—you look at how you lower the overall energy of the system. That's a time-averaged perspective.

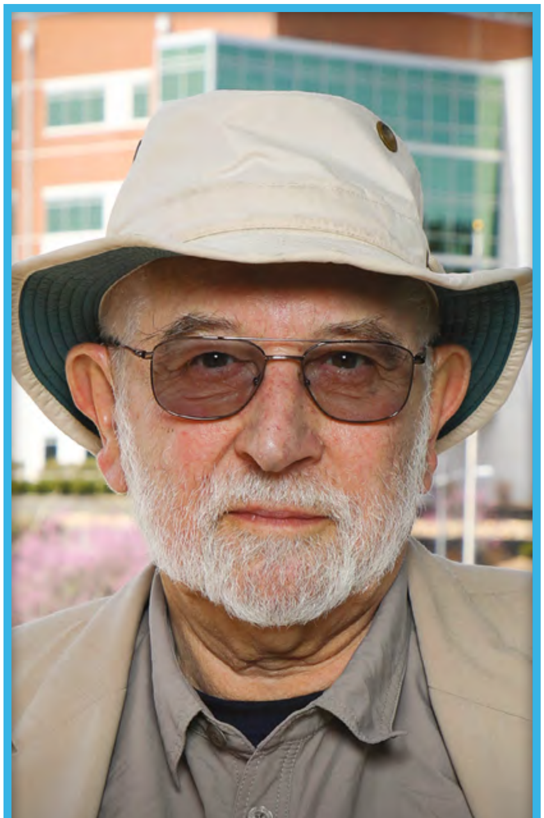
What we are looking to do is understand how these processes occur *in situ*; and then on the ultrafast time scale, how do they hold onto molecules, how do they dissipate energy in very efficient ways.

The idea is that if you understand those time-dependent kinetic aspects of the chemistry, you can then design molecules that will better funnel energy into keeping a bond intact; or you can better design molecules that will aggregate or self-assemble in ways that target a molecule that you want selectively.

4. What attracted you to a career in science?

The first time I was really interested in science, I was at a diner with my dad, and he was telling me about relativity, of all things. We were just chatting, and he told me about a book, *A Brief History of Time*, by Stephen Hawking, that I then read, and it got me interested in physics.

Then I went to college, mostly because I didn't want to pay for rent. If I didn't go to college, he was going to make me pay rent at home, so I went and signed up for college. I did that, and I was good at chemistry, and I just kind of kept going. It was one of those things that, once that ball got going, it was fairly easy to stay in it.



Michael Berry is the Melville Wills Professor of Physics Emeritus at the University of Bristol, United Kingdom.

A fellow of the Royal Society of London and a foreign associate of the National Academy of Sciences, Berry has received numerous awards including the Moët Hennessey-Louis Vuitton Science for Art prize, the Wolf Prize in Physics and the Lorentz Medal of the Royal Netherlands Academy of Arts and Sciences.

He holds 13 honorary degrees from universities around the world and serves on advisory committees for the International Institute for Physics, Natal, Brazil, and the Harvard Center for Mathematical Sciences and Applications. He is a member of the Institute for Quantum Studies at Chapman University, Orange, California, and serves on the International Board of the Weizmann Institute of Science, Rehovot, Israel.

On April 5, 2018, Berry delivered the Eugene P. Wigner Distinguished Lecture on the topic "Making Light of Mathematics." His talk reflected on Wigner's 1960 paper, "The Unreasonable Effectiveness of Mathematics in the Natural Sciences." This is an edited transcript of our conversation following his lecture.

Distinguished

Michael Berry

1. How do visually stunning and beautiful phenomena such as rainbows or twinkling starlight illustrate the value of mathematics?

It was known for centuries—Galileo emphasized it—that if we want to understand the physical world, the natural language is mathematics.

Many of the things we discover and we study in science are things that you can't perceive directly. Nobody's seen an atom. Nobody's felt a gravity wave pass by. So, the relationship between the mathematics and the phenomenon is often quite obscure. We scientists understand the principle of it, but not always the details.

But with some visual phenomena, like rainbows and the sparkling of the sun on the sea, you can describe the mathematics in a way that directly relates to what people see, and that's helpful.

2. How are these concepts useful for promoting science and research?

They say a picture is worth a thousand words. That's true, but as scientists we know that an equation summarizes, economically, infinitely many pictures. So why do we need pictures? The reason is that the extreme compactness of equations makes it hard to understand what they contain. Pictures can help make that clear to people. So I think pictures are as important as visual phenomena that you can see directly.

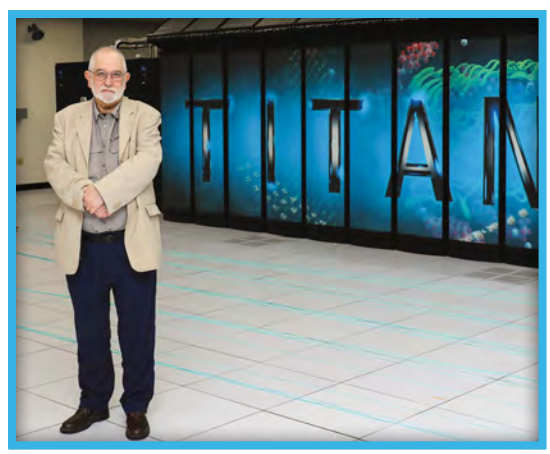
3. How do these concepts echo Wigner's article "The Unreasonable Effectiveness of Mathematics in the Natural Sciences"?

In a curious way. In that article, there are very many sensitive observations about how the mathematics that's in our heads is related to the world that's outside.

But I don't quite agree with him. He's talking about the unreasonable effectiveness as though there's no reason why that should happen. But I think there is a reason. We are creatures recently evolved. We haven't been around for more than a tiny sliver of cosmic time. We are still developing. We know a little more than dogs, but not that much more in the grand scheme of things.

We understand bits and pieces of this inscrutable universe. How? We can only understand what we are capable of understanding. Thus, we can only understand those aspects of the universe that reflect the most sophisticated constructs that our minds can make.

Lecturer



What are those constructs? They are mathematical. So, it's inevitable that the most recent mathematics is going to find its echo—or be necessary—in order to understand things in the physical world.

Sometimes, the maths comes first—almost as though it's waiting for us. Einstein had learned that there is something called the geometry of curved spaces. Nobody thought it was any use, but there it was, just waiting for him to pick it up and use it in his gravity theory. Sometimes, physicists do the mathematics first, and the mathematicians then elaborate it. But whether the physics or the mathematics comes first, it seems inevitable that sophisticated mathematics would describe aspects of the universe. It's because of the way we are made. So, I don't think the effectiveness of mathematics is unreasonable; I think it's inevitable. But it is wonderful!

4. Machine learning and artificial intelligence are able to find patterns in data without a mathematical underpinning. What does that say about the role of mathematics in future scientific research?

Machine learning is relatively recent, and within physics it hasn't yet contributed much that is fundamental. There are some interpretations of data and detection of patterns in pictures. My reaction is that although it's a different kind of discovery, once you see the patterns, you want to understand them, and then you need maths again.

5. Why was it important to visit ORNL, meet with researchers here, and participate in the Wigner Lecture Series?

For me the main reason is, what an honor! We all have boundless admiration for Wigner, and to be associated even in this way with his name is a wonderful thing. Of course, it's intimidating, given the list of all the people who came before. Visiting ORNL is like visiting any other excellent place where scientific research is done. You meet people you don't know. You learn surprising things. And you take them away with you. ORNL is indeed a place of great excellence. It's part of the great patchwork of organizations where great science is done.

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.

ORNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished staff members, 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.

Juliane Weber

Postdoc, Chemical Sciences Division
Ph.D., Geosciences, RWTH Aachen University, Germany
Hometown: Bonn, Germany

What are you working on at ORNL?

I am a geochemist, and I focus on understanding the fate of harmful materials such as heavy metals or radionuclides at the environmentally relevant mineral-water interface over different length scales. For this, I combined experimental wet-chemistry with different high-resolution chemical imaging characterization techniques such as atom probe tomography.

What would you like to do in your career?

I would like to build a research program to investigate what controls mineral reactivity and then understand how we can use this knowledge to immobilize harmful elements, e.g., radionuclides or heavy metals, and, as a consequence, make energy production more efficient and environmentally friendly.

Why did you choose a career in science?

I like to be challenged intellectually every day—which is guaranteed when working in science. In addition, I love to contribute my part to humankind's effort to understand the underlying principles of how things work in nature and how we can make use of these principles in our everyday lives.

Carlos Andres Polanco

Postdoc, Materials Science and Technology Division
Ph.D., Electrical Engineering, University of Virginia
Hometown: Bogota, Colombia

What are you working on at ORNL?

My work focuses on understanding and modeling how thermal energy flows across interfaces and crystalline materials with defects. Combining the intuition gained with predictive models—free from fitting parameters—I design novel materials with targeted thermal properties to enhance the performance of devices for energy applications.

What would you like to do in your career?

I want to push the boundaries of our fundamental understanding of the motion of thermal energy and use that new knowledge to engineer the next generation of energy solutions—that is, materials and devices that can better harvest, dissipate or control thermal energy. Thermal energy is abundant but challenging to control!

Why did you choose a career in science?

Since I was a kid, I wanted to understand how "magic" devices work—how a light bulb shines, how a plane flies, how a computer runs a program. This curiosity turned into personal satisfaction as my first physics classes started uncovering the tricks.

Patricia Blair

Postdoc, Biosciences Division
Ph.D., Chemistry, University of Illinois at Urbana-Champaign
Hometown: Lenexa, Kansas

What are you working on at ORNL?

In the Plant-Microbe Interfaces Science Focus Area, we study organisms living in the plant microbiome and how those organisms interact with one another as well as with the host plant. Specifically, I study signaling molecules and antibiotics that soil-dwelling bacteria produce in order to colonize plants and prevent disease.

What would you like to do in your career?

I aim to plan and implement scientific research for the government, applying analytical and environmental chemistry as well as chemical biology to better understand the natural environment as well as the effects of human society on the environment.

Why did you choose a career in science?

While my main motivation for studying science is my faith, I also find science challenging and satisfying as a discipline. The challenging problems motivate me to work diligently and learn constantly, and the endless supply of questions to be answered fosters my curiosity about the natural world.

Riddhi Shah

Graduate student, Neutron Scattering Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Ahmedabad, India

What are you working on at ORNL?

The goal of my research is to understand polymer interactions and structural changes that occur between the components of the plant cell wall during thermochemical processes. This knowledge would eventually help produce biofuels efficiently. I also design and construct systems mimicking plant cell walls in order to probe polymer interactions that are not easy to study in plant cell walls.

What would you like to do in your career?

My passion has been structural studies on biological systems like plant cell walls, proteins and enzymes and correlation of the structure with its function in order to improve its function or make bioproducts. I would like to continue to be a part of research related to this either in an industrial or academic setting.

Why did you choose a career in science?

My schoolteachers played an important role in shaping my thought process and in making me like science. As I grew older, forming hypotheses and designing experiments to solve science-related problems interested me a lot, and this made me choose a career in science.

Swapnil Desai

Graduate student, Computational Sciences and Engineering Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Valsad, Gujarat, India

What are you working on at ORNL?

I am working on direct numerical simulations of multistage mixed-mode turbulent combustion using high-performance computing to elucidate the key physics that govern autoignition and flame stabilization under the conditions of next-generation engines which operate near combustion limits to maximize efficiency and minimize harmful emissions.

What would you like to do in your career?

After graduation, I intend to join an organization where I can continue my work on the development of science-based computational applications that effectively utilize high-performance computing technology to provide breakthrough simulation and data analytic solutions for the efficient and responsible production and use of energy to meet the growing needs of the world.

Why did you choose a career in science?

I've always been curious about how things worked. We live in a technological world, and its complexity continues to throw up challenges. Some are life and death, like finding energy sources that mitigate climate change or predicting when and where a hurricane will make landfall. The fascination of finding and sometimes predicting the right answers makes being in science worthwhile.

Kristine Grace Manno Cabugao

Graduate student, Environmental Sciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Hercules, California

What are you working on at ORNL?

I study plant and microbial interactions related to phosphorus cycling in tropical forests as part of the Next Generation Ecosystem Experiments Tropics project. Understanding the link between root functional traits, the surrounding microbial community, and soil provides data for ecosystem models about how belowground processes influence the tropical carbon sink.

What would you like to do in your career?

I have always seen science and policy as complementary, and I know that what drew me to the Bredesen Center and the Climate Change Science Institute was their interdisciplinary nature. After my dissertation, I hope to pursue a career that merges science and policy, ideally within international development.

Why did you choose a career in science?

I asked for a microscope when I was a kid—the red one from Toys "R" Us. And the first time I thought about being a scientist was when I isolated DNA in high school. I was fascinated by how the smallest aspects of life could influence what we observe.

We won the war. What's next?

by Tim Gawne
gawnetj@ornl.gov

While V-J Day in August 1945 heralded the end of World War II for most of the country, it brought uncertainty to many of the men and women of the Manhattan Project.

They had been part of history's greatest technological crash course—creating the first nuclear weapons less than seven years after the discovery of nuclear fission—but when the Manhattan Project ended, so did their draft deferments. Some, in fact, were sent to Germany and Japan as part of the post-war occupation.

The uncertainty had begun before the war's end. The Army's priority in the final months of the project was clear: Maintaining a modest R&D capability while pushing production as fast as possible. As a result, many junior scientists found themselves unexpectedly drafted into Uncle Sam's army and released from the project. The Trinity test—the first detonation of a nuclear bomb—was an enormous technical accomplishment but also accelerated the shift away from the R&D that was essential in early pursuit of the bomb.

Some project sites went on standby. The X-10 site in Tennessee, however, had the fortune of being able to troubleshoot production issues at the Hanford site in Washington state and to assist research at the Los Alamos lab in New Mexico. As a result, X-10—later to become ORNL—remained fully staffed and funded.

For scientists, the Manhattan Project had not been about the bombs as much as it had been about the research. Nuclear science, which enjoyed the freshly minted term "nucleonics," cut across long-established fields from physics to biology and held so much promise that it marked the beginning of a new era for science and civilization: the "Atomic Age."

Aerial view of ORNL in the late 1940s. Image credit: ORNL

X-10 wanted a piece of that action. Its leaders saw the lab as a center of excellence and an anchor to universities across the Southeast, yet a visitor could be forgiven for seeing only dust, mud and temporary structures. There was no guarantee it would survive the peace.

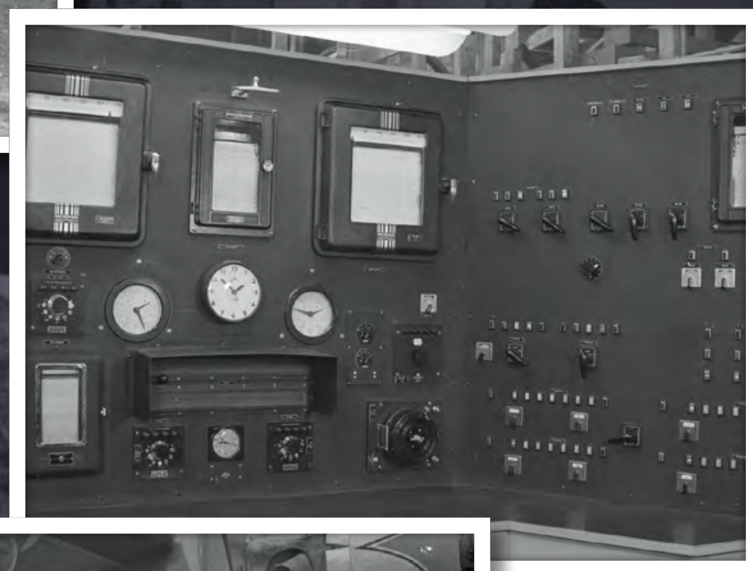
The lab remained in limbo—through leadership changes, shifting programs and priorities, and the transfer of control from the Army to the civilian Atomic Energy Commission—until 1948, when its survival was finally assured.

At one point, there was even a push to move X-10 to the Y-12 site one valley over. Fortunately, cooler heads prevailed when they contemplated the cost of decommissioning and rebuilding the lab's Graphite Reactor.

ORNL owes its existence to a few key individuals—such as William Pollard, Eugene Wigner and Alvin Weinberg—who made it their life's mission to ensure that the Tennessee laboratory survived and flourished. That Graphite Reactor—the world's first continuously operating reactor—advanced many fields of study, including several that remain strengths of ORNL such as neutron science, biology and genetics, chemistry and materials science.

It was also the world's largest producer of stable isotopes and radioisotopes. As an old newspaper headline put it dramatically: "Out of the fire of hell comes the cure for cancer!"

An ORNL public relations photo from the late 1940s. Image credit: ORNL



The Graphite Reactor control panel (1944). Image credit: ORNL

A shipment of isotopes is transferred to American Airlines at the Knoxville Airport in 1947. Image credit: ORNL

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