OAK RIDGE NATIONAL LABORATORY

Review

18 · Farewell, Titan!

28 · Harvesting uranium

32 · Honoring talented young researchers

Neutrons to the rescue:

10 · Researchers explore materials at the atomic scale

Oak Ridge National Laboratory

Vol. 53 | No. 1 | 2020

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Contents

On the Cover

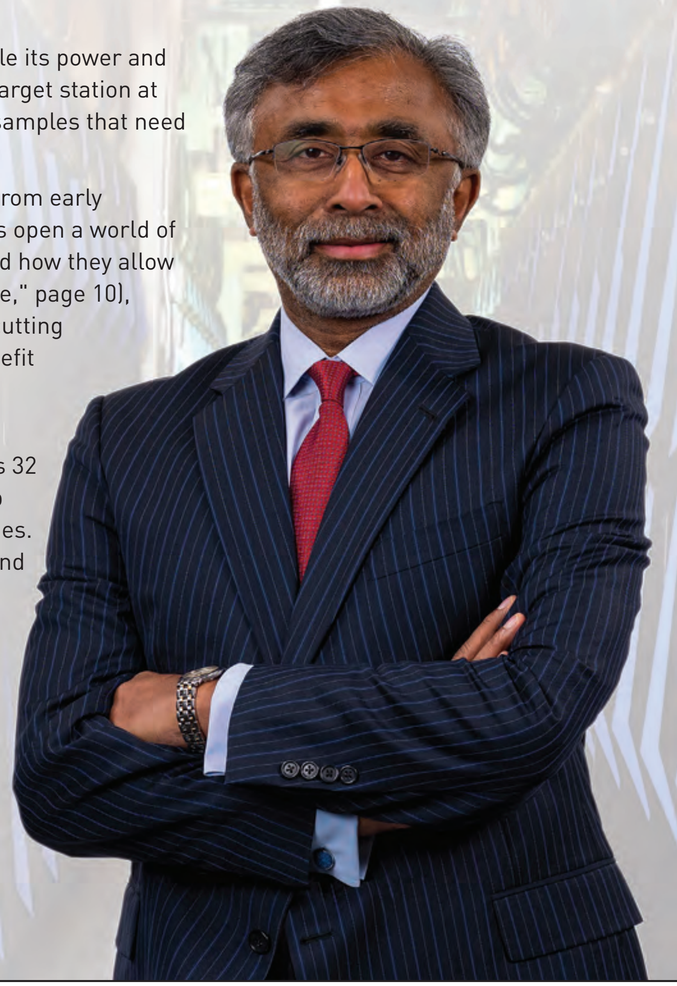
Neutron scattering scientist Hugh O'Neill leads ORNL's Center for Structural Molecular Biology.
Image credit: Genevieve Martin, ORNL

Neutron scattering for a better world

Neutron science began at Oak Ridge in 1944 when researcher Ernest Wollan took advantage of the world's first continuously operating nuclear reactor—the X-10 Graphite Reactor—to study the diffraction of neutrons in a single crystal.

In the intervening years, neutron scattering has proved to be an indispensable tool for scientific research, with neutron research at ORNL leading the way to such advances as better batteries, more effective drugs, and stronger armor for the military. The ability of neutrons to probe the magnetic properties of materials, to interact with light elements and to travel through materials that would stop X-rays or an electron beam make neutron scattering ideal for research areas ranging from quantum materials to biological systems to industrial applications in energy storage, automotive, aerospace and much more.

Seven and a half decades after Wollan's groundbreaking work, ORNL is still at the forefront of neutron scattering research with two world-class facilities: the accelerator-based Spallation Neutron Source, which provides the world's most intense pulsed neutron beams, and the High Flux Isotope Reactor, which provides one of the highest rates of continuous-beam neutrons of any research reactor in the world.



In the coming years, an upgrade to the SNS proton accelerator will double its power and increase the flux (quantity of neutrons) produced by SNS, and a second target station at the facility will add new research capabilities in complex materials and samples that need high resolution over a wide range of length and time scales.

In this issue of *ORNL Review*, we look at the history of neutron research from early efforts to understand the atom to the present and beyond (see "Neutrons open a world of research," page 8), we explore the unique characteristics of neutrons and how they allow us to expand our knowledge (see "What makes neutron scattering unique," page 10), and we explain how upgrades at SNS will keep the United States at the cutting edge of neutron research for years to come (see "SNS upgrades will benefit researchers," page 12).

Elsewhere in this issue, we profile nine extraordinary young researchers who have received prestigious early-career awards (see stories on pages 32 through 41). Seven received the DOE Early Career Research Award, a lab record and over a quarter of the 27 awarded to the 17 national laboratories. Two others received the Presidential Early Career Award for Scientists and Engineers, the U.S. government's highest honor for scientists and engineers in the early years of their careers.

Also in this issue, we honor ORNL's Titan supercomputer, which was decommissioned this past August (see "Farewell, Titan: A long-running supercomputer with tremendous impact," page 18). Titan debuted as the world's fastest system in 2012, and as late as last June was ranked as high as number 12 in the world. Among its many achievements, it advanced the production of cellulosic ethanol and helped Southern California prepare for future earthquakes.

I hope you enjoy reading about ORNL's contributions to neutron science and other important research stories from around the lab.

Thomas Zacharia

Thomas Zacharia
Laboratory Director

New US director named for ITER fusion reactor

Kathy McCarthy has been named director of the US ITER Project Office at ORNL, effective March 2020.

Kathy McCarthy

US ITER is managed by ORNL, with partner labs Princeton Plasma Physics Laboratory and Savannah River National Laboratory, and has the responsibility of designing, fabricating and delivering hardware for ITER, the international experimental reactor under construction in France. ITER's goal is to produce and study a burning plasma, an important step for fusion energy development.

"Kathy is a proven scientific leader who combines technical expertise with experience successfully managing large and complex organizations," ORNL Director Thomas Zacharia said.

McCarthy joins ORNL after three years as vice president for science and technology and laboratory director for the Canadian Nuclear Laboratories, where she has overseen a staff of 650 and grown the labs' commercial work. She previously held a variety of engineering and leadership roles at Idaho National Laboratory, including director of domestic programs in INL's Nuclear Science and Technology Directorate, director of the Light Water Reactor Sustainability Program Technical Integration Office, and national technical director for the Systems Analysis Campaign for the DOE Office of Nuclear Energy's Fuel Cycle R&D Program.

McCarthy succeeds Ned Sauthoff, who is now advising lab-wide efforts across the ORNL research portfolio.—*Morgan McCorkle*

ORNL fuel tech may boost ethanol

A technology developed at ORNL and scaled up by California-based Vertimass LLC to convert ethanol into fuels suitable for aviation, shipping and other heavy-duty applications can be price-competitive with conventional fuels while retaining the sustainability benefits of bio-based ethanol, according to a new analysis.

ORNL worked with technology licensee Vertimass and researchers at 10 other institutions on a technoeconomic and life cycle sustainability analysis of the process—single-step catalytic conversion of ethanol into hydrocarbon blendstocks that can be added to jet, diesel and gasoline fuels to lower their greenhouse gas emissions. This new technology is called Consolidated Dehydration and Oligomerization, or CADO.

A pilot reactor, developed by Vertimass and located at TechnipFMC, can scale up the process that converts ethanol into fuels suitable for aviation, shipping and other heavy-duty applications. Credit: TechnipFMC

The analysis, published in the *Proceedings of the National Academy of Sciences*, showed that this single-step process for converting wet ethanol vapor could produce blendstocks at $2 per gigajoule today and $1.44 per gigajoule in the future as the process is refined, including operating and annualized capital costs. That would make the blendstock competitive with conventional jet fuel produced from oil at historically high prices of about $100 per barrel. At $60 per barrel, the use of existing renewable fuel incentives results in price parity, the analysis found.—*Stephanie Seay*

ORNL researchers picked for grid modernization

ORNL researchers will lead two new projects and support seven more to enhance the reliability and resilience of the nation's power grid as part of DOE's 2019 Grid Modernization Lab Call.

DOE announced funding of approximately $80 million over three years for 23 projects across the country. ORNL is expected to receive approximately $10 million of available funding to support the nine projects on which it collaborates.

This latest round builds upon two previous solicitations released in 2016 and 2017 by the Grid Modernization Initiative, providing a continued focus on reliability and resilience. The research brings together scientists from DOE's national labs with industry and university partners to develop efficient, cost-effective solutions to harden the grid against disruption and to make it more resilient when events occur. The projects address challenges that range from power generation to transmission across vast distances to the local distribution of electricity by utilities.

"We are proud to be a part of the Grid Modernization Initiative and bring our world-class expertise for providing innovative technology solutions to fortify the nation's electricity delivery system," said

Moe Khaleel, associate laboratory director for energy and environmental sciences at ORNL. "A modern, resilient power grid is vital to the nation's economic and national security and to the well-being of its citizens."

ORNL will lead two projects. In the first, the Multi-Port Modular Medium-Voltage Transactive Power Electronics Energy Hub, researchers will design and develop medium-voltage power electronics hardware and software to enable the integration of the growing volume of intermittent, renewable energy sources into the grid while ensuring the smooth flow of electricity. The second, Vulnerability of Power Generation Critical Systems Against Electromagnetic Threats, will experimentally evaluate the physical security of power generation plants against electromagnetic threats.—*Stephanie Seay*

Paranthaman gets top ORNL science award

Parans Paranthaman, a researcher in ORNL's Physical Sciences Directorate, has received the ORNL Director's Award for Outstanding Individual Accomplishment in Science and Technology for his efforts in mentoring and developing future scientists.

The Director's Awards were presented by ORNL Director Thomas Zacharia during the annual Awards Night event hosted by UT-Battelle, the management and operating contractor of ORNL for the Department of Energy.

Paranthaman received the laboratory's top science and technology award "for teaching and mentoring more than 56 undergraduate and graduate students during the past eight years to be their best, strengthen their critical thinking abilities, and develop research skills for success in graduate school and future jobs." He also received the Mentor of Student Researchers award at the ceremony.

Paranthaman, an ORNL Corporate Fellow and leader of the Chemical Sciences Division's Materials Chemistry Group, 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. He is a fellow of multiple professional societies and holds numerous patents related to superconductivity, energy storage and solar cells.—*Bill Cabage*

Parans Paranthaman

'Highly Cited Researchers' list includes 9 from ORNL

Nine ORNL scientists have been named to the 2019 Highly Cited Researchers list released by the Web of Science Group.

The list identifies scientists who produced multiple papers ranking in the top 1 percent by citations for their field and year of publication over the last decade, demonstrating significant research influence among their peers.

This year's listing includes the following researchers from ORNL:

- Sheng Dai of the Chemical Sciences Division
- Colleen Iversen of the Environmental Sciences Division
- Peter Maksymovych of the Center for Nanophase Materials Sciences
- David Mandrus, joint faculty with the University of Tennessee
- Michael McGuire of the Materials Science and Technology Division
- Richard Norby of the Environmental Sciences Division
- Peter Thornton of the Environmental Sciences Division
- Gerald Tuskan, director of the Center for Bioenergy Innovation
- Jiaqiang Yan of the Materials Science and Technology Division

"This recognition exemplifies the leading contributions the laboratory's scientists are making to the community of science and the importance of that research in fields such as chemical, biological, environmental and materials sciences," ORNL Deputy for Science and Technology Michelle Buchanan said.—*Morgan McCorkle*

ORNL scientists have developed an experiment for testing potential materials for use in interplanetary travel. The experiment exposes prototype materials to temperatures over 2,400 degrees Celsius with only 300 watts of input electrical power. Image credit: Carlos Jones, ORNL

Experiment tests materials for reactor-based rockets

If humankind reaches Mars this century, an ORNL-developed experiment testing advanced materials for spacecraft may play a key role.

NASA is considering nuclear thermal propulsion—powering spacecraft with a nuclear reactor, which could cut travel times in half compared to traditional rockets. A nuclear-fueled system will need sophisticated materials that can withstand extreme temperatures, hydrogen propellant and radiation.

ORNL's experiment exposed prototype components to electrically heated temperatures reaching over 2,400 degrees Celsius. Soon, scientists will take a scaled-up version containing fuel surrogates and instrumentation to the Ohio State University Research Reactor to see how it fares when neutron irradiation is added.

"There's nothing out there like this," ORNL's Richard Howard said. "We've built a remarkably efficient platform for reproducing extreme temperatures, and we're confident the scaled-up version will perform just as well."

Future work may include an even larger version to test full-size fuel elements or other reactor components.—*Jason Ellis*

ORNL researchers receive five R&D 100 Awards

ORNL researchers have received five 2019 R&D 100 Awards, increasing the lab's total to 221 since the award's inception in 1963.

Known as the "Oscars of Invention," the awards recognize the top 100 revolutionary technologies of the year, as well as the scientists and engineers who created them. ORNL researchers received awards for the following innovations:

CellSight—Rapid, Native Single Cell Mass Spectrometry, developed by ORNL and Cytena GmbH. Knowing the broad chemical makeup of a single cell can advance disease diagnosis and more effective therapeutics. In medicine, pharmaceuticals and environmental monitoring, there is a need to detect, target and chemically characterize cellular subpopulations in their native environment.

To meet this need, ORNL researchers have developed CellSight, which enables rapid mass spectrometry of individual cells. The product ejects tiny droplets of liquid solution containing single cells through a mechanism similar to an inkjet printer head. The cell is imaged, isolated and then transferred to the mass spectrometry system, where CellSight's unique software delivers quick analysis.

The ORNL team was led by John Cahill and included Vilmos Kertesz.

High Strength Binder System for Additive Manufacturing, developed by ORNL and ExOne. Binder jetting is an additive manufacturing technology that works by layering powdered materials and cohering them into desired shapes using a liquid binding material deposited via inkjet. Though these liquid binders are vital ingredients in the binder jetting process, few improvements have been made on binder technology in recent decades.

ORNL researchers have developed a novel liquid binder that is stronger, more functional and more environmentally friendly than the most widely used liquid binder, furan. The binder can be deposited in large quantities while also maintaining sharp features in an object's design, meaning the strength can be finely tuned to its applications. Parts printed with the binder can be stronger than cement.

Tomonori Saito and Amy Elliott led the ORNL team, which included ORNL's Lu Han as well as Dustin Gilmer and Michelle Lehmann of the University of Tennessee's Bredesen Center for Interdisciplinary Research and Graduate Education.

Multiparameter Sensor Platform for Cyber-Physical Security of the Electric Grid, developed by ORNL and Brixon. ORNL researchers have developed multiparameter sensor platforms that can communicate with utility operators and provide real-time surveillance of the electric grid. Called grid agents, these devices can help improve situational awareness and protect the grid from cyber-physical attacks.

The sensors have an important dual function. They can monitor several physical parameters related to grid operations, including temperature, solar irradiance and chemical gases such as methane and hydrogen. Simultaneously, they relay network communications back to a utility's IT security system, helping utilities optimize grid function and ensure security.

The ORNL team was led by Peter Fuhr and included Marissa E. Morales-Rodriguez, Gary Hahn, Kenneth Woodworth and Sterling Rooke.

Voltanol: Electrochemical Conversion of Carbon Dioxide to Ethanol, developed by ORNL. A team of ORNL researchers has developed a carbon nanospike catalyst—a nanotechnology-based electrocatalyst composed of carbon, nitrogen and copper—that can convert carbon dioxide and water to ethanol. The catalyst is made of a highly textured form of graphene—a type of single-layer carbon—that is arranged into atomically sharp spikes embedded with copper nanoparticles. Together they form a sequential catalyst that synthesizes ethanol.

Ethanol is an affordable, high-energy–density liquid fuel that could be a viable alternative to gasoline for internal combustion engines. Converting water and waste CO_2 to ethanol also removes the harmful greenhouse gas from the air. Using renewable electricity to power the reaction makes the process carbon-neutral.

ORNL's Adam Rondinone and Yang Song, formerly of ORNL, led the development team, which also included ORNL's Dale Hensley and Peter Bonnesen.

In addition, ORNL worked as a partner on **Unified Communications X (UCX)**, submitted by Los Alamos National Laboratory and codeveloped by Arm Ltd., Mellanox Technologies, ORNL, Advanced Micro Devices, Argonne National Laboratory, NVIDIA, Stony Brook University and Rice University.

As supercomputers worldwide move toward exascale—the ability to complete a quintillion calculations per second—they increasingly incorporate diverse hardware and processing systems. For all of the elements in these systems to operate harmoniously, they must communicate.

UCX is an open-source software for high-performance computers that allows these hardware systems and architectures to communicate by creating common interface definitions. By defining a common set of features between hardware and programming models, UCX allows developers to bind together libraries, network architectures and custom software and hardware interfaces into one package, essentially channeling the diversity of the world's HPC applications into one user-friendly research tool.—*Abby Bower*

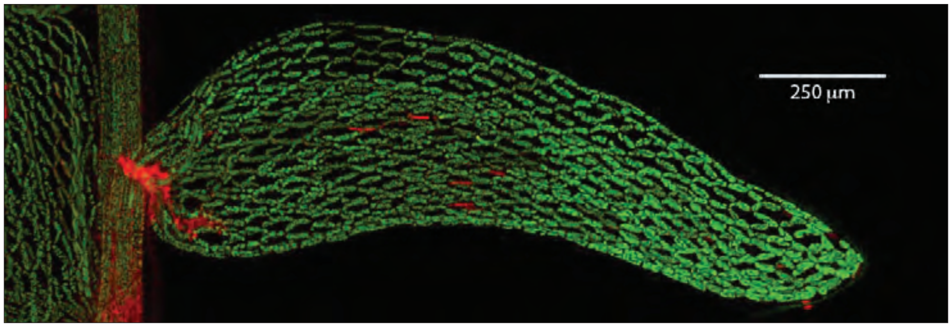
Warming temps break down moss–microbe interactions

Scientists from ORNL and Georgia Tech found that critical interactions between microbes and peat moss break down under warming temperatures, impacting moss health and—ultimately—carbon stored in soil.

The team investigated the mosses' reaction to a range of temperatures onsite at SPRUCE—the Spruce and Peatland Responses Under Changing Environments experiment—a whole-ecosystem warming experiment in the peatlands of Minnesota. Using genomic analyses, the team showed that the heat caused microbial diversity to decline, reducing the microbiome's ability to capture nitrogen from the air for moss to use.

"*Sphagnum* mosses and their microbiomes substantially control the cycling of carbon and nitrogen across the landscape," ORNL's David Weston said. "We are looking at what is causing this breakdown in the relationship between mosses and microbes."

This research advances our understanding of how changing environmental conditions might affect nearly one-third of the world's soil organic carbon currently stored in northern peatland ecosystems.—*Kim Askey*



Beneficial microbes, shown in red, aid Sphagnum *mosses in using nitrogen from the air to fuel plant growth. ORNL scientists have shown this nitrogen-fixing activity declines with warming temperatures.* Image credit: David Weston, ORNL

Researchers at the Center for Nanophase Materials Sciences at ORNL demonstrated an insect-inspired, mechanical gyroscope to advance motion-sensing capabilities in consumer-sized applications. Credit: Jill Hemman, ORNL

Miniaturized gyroscope inspired by flying insects

Researchers at ORNL and the National Renewable Energy Laboratory in Colorado took inspiration from flying insects to demonstrate a miniaturized gyroscope, a special sensor used in navigation technologies.

Gyroscopes sense rotational motions to provide directional guidance without relying on satellites, so they are immune to signal jamming and other cyber threats. This makes them ideal for aircraft and submarines.

Integrating the devices into smaller defense and consumer electronics has been challenged by fundamental obstacles. At micro sizes, gyroscopes' electrical components can produce noise that interferes with their operation. To maintain performance at microscale, the research team developed an all-mechanical device with no on-chip electrical components.

The coin-sized design, fabricated at the Center for Nanophase Materials Sciences at ORNL, mimics halteres, the vibrating wing-like organs flying insects use to navigate.

"Our goal was to optimize cost and performance in the smallest design possible to expand the market for this technology," ORNL's Nick Lavrik said.—*Ashley Huff*

Gina Tourassi to lead ORNL computing division

Gina Tourassi has been appointed director of the National Center for Computational Sciences, a division of ORNL's Computing and Computational Sciences Directorate.

Gina Tourassi

The NCCS is home to the Oak Ridge Leadership Computing Facility, which houses Summit, the world's most powerful supercomputer.

Tourassi first joined ORNL in 2011 in the Computational Sciences and Engineering Division as the founding director of the ORNL Health Data Sciences Institute and most recently served as the group leader of ORNL's Biomedical Sciences, Engineering, and Computing Group.

Before coming to ORNL, she held numerous academic positions at Duke University Medical Center. Her prolific scientific efforts have produced 11 patents and invention disclosures and a 2014 R&D 100 award, as well as more than 250 peer-reviewed journal articles, conference proceedings articles, and book chapters.

"Gina was chosen from an outstanding pool of candidates for her dedication to world-class research," said Jeff Nichols, ORNL's Computing and Computational Sciences associate laboratory director. "Gina has used her interdisciplinary expertise at the intersection of artificial intelligence and applied data sciences to spearhead rapid growth of the Laboratory's capabilities in biomedical sciences and engineering."

With OLCF Program Director Buddy Bland and OLCF-5 Project Director Justin Whitt, Tourassi will lead the division as it continues to prepare for installation and the 2021 launch of Frontier, one of America's first exascale supercomputers, which will be able to perform more than a quintillion calculations a second.—*Andrea Schneibel and Katie Bethea*

Metal foam may boost eco-friendly refrigerants

ORNL researchers have demonstrated that metal foam enhances the evaporation process in thermal conversion systems and enables the development of compact heating, ventilation, air conditioning and refrigeration, or HVAC&R, units.

Compact and efficient HVAC&R equipment is needed to support the global industry transition to alternative, environmentally friendly refrigerants. The small-scale evaporator proved metal foam is well-suited for compact systems.

"We found that the presence of a porous open cell or sponge-like metal foam layer in an evaporator's tubes increases the liquid refrigerant's boiling rate, creating essentially an enhanced pool-boiling process that can accommodate much higher heat fluxes compared to conventional technology," ORNL's Kashif Nawaz said. "Enhancement materials like metal foams increase equipment efficiency by improving the phase change or vaporization process."—*Jennifer Burke*

Polymer protects planes from lightning strikes

ORNL researchers have demonstrated that an additively manufactured polymer layer, when applied to carbon-fiber–reinforced plastic, or CFRP, can effectively protect aircraft against lightning strikes.

CFRP is typically used on an airplane's exterior because it's lighter than traditional metal. Although lightweight, CFRP has drawbacks—low electrical conductivity and heat resistance—making it vulnerable to lightning strikes.

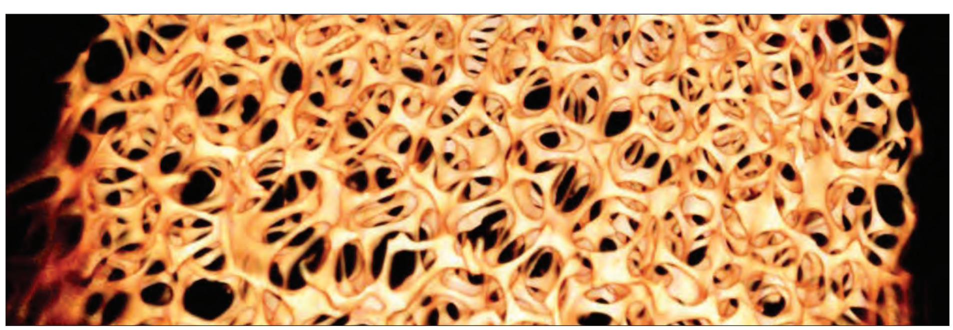
"We printed a novel, easy-to-apply adhesive material for CFRP," ORNL's Vipin Kumar said. "The polymer's chain-like structure makes the resulting material electrically conductive and structurally strong with thermal treatment."

In a study, the research team conducted simulated lightning strike tests on CFRP, both with and without polymer protection.

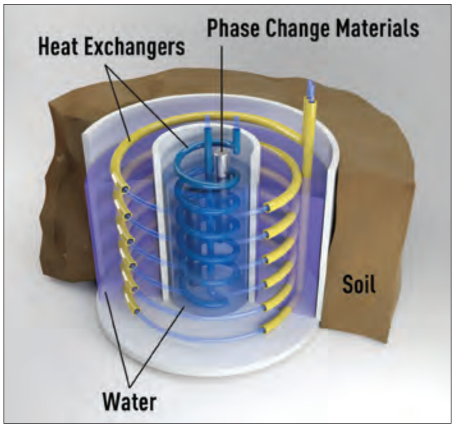
"The polymer-protected sample showed minimal damage upon visual inspection and enabled much more uniform heat dissipation," Kumar said. "Our results proved that the polymer layer provided a continuous path to effectively distribute the lightning current."—*Jennifer Burke*

Geothermal storage can save electricity

ORNL researchers have created a geothermal energy storage system that could reduce peak electricity demand up to



ORNL researchers discovered that open cell metal foams have complex cell structure and a large surface per unit volume, which enhance the pool-boiling process necessary for evaporation in HVAC&R units. They developed a small-scale evaporator to prove the foams could function well in complex systems. Image credit: Kashif Nawaz, ORNL



ORNL researchers have developed a system that stores electricity as thermal energy in underground tanks, allowing homeowners to reduce their electricity purchases during peak periods while helping balance the power grid. Image credit: Andy Sproles, ORNL

37 percent in homes while helping balance grid operations.

The system is installed underground and stores excess electricity from renewable resources like solar power as thermal energy through a heat pump. The system comprises underground tanks containing water and phase change materials that absorb and release energy when transitioning between liquid and solid states.

ORNL's design relies on inexpensive materials and is installed at shallow depths to minimize drilling costs. The stored energy can provide hours of heating in the winter or cooling in the summer, shaving peak demand and helping homeowners avoid buying electricity at peak rates.

"Shifting demand during peak times can help utilities better manage their loads while saving consumers money and encouraging greater use of renewable energy," said ORNL's Xiaobing Liu.—*Stephanie Seay*

Energy use simulation helps quantify savings

To better determine the potential energy cost savings among connected homes, ORNL researchers have developed a computer simulation to more accurately compare energy use on similar weather days.

"Since no two weather days are alike, we created a simulated weather identification model that keeps environmental impacts such as temperature changes and sunlight consistent," ORNL's Supriya Chinthavali said. "This will help address the challenge of quantifying energy cost savings, which utility companies and homeowners are most interested in."

The team is analyzing energy use data from a neighborhood-level research platform comprising 62 homes called Smart Neighborhood in Hoover, Alabama, powered by traditional electric grid and microgrid sources.

The goal is to co-optimize energy cost, comfort, environment and reliability by controlling the connected homes' devices—particularly the HVAC and water heater, a home's largest energy consumers.

Future analysis by ORNL, Southern Company and university partners will include potential energy cost savings details.—*Sara Shoemaker*

Wireless charger designs boost power density

New designs created and tested by ORNL researchers may double the power density of wireless chargers, paving the way for lighter chargers that are nevertheless safe.

The hands-free method includes a set of two charging coils—one affixed underneath an electric vehicle and the other at ground level. When the coils are aligned, the power that is transferred charges the vehicle's battery.

The team's designs—described recently in the journal *IEEE Transactions on Power Electronics*—include a three-phase system that features rotating magnetic fields between layers of coils.

"The layered coil design transfers power in a more uniform way, allowing for an increase in power density," ORNL's Jason Pries said.

The three-phase system has successfully transferred 50 kilowatts with 95 percent efficiency. "As we scale up the system to transfer up to 300 kilowatts, the specific power is expected to improve as well."

This research brings the team another step closer to fully charging an EV in 20 minutes.—*Sara Shoemaker*

ORNL's Ozpineci named IEEE fellow

ORNL researcher Burak Ozpineci has been elevated to fellow of the Institute of Electrical and Electronics Engineers. The IEEE cited Ozpineci for his "contributions to transportation electrification and wireless charging of electric vehicles."

Burak Ozpineci

Ozpineci directs the Electric Drive Technologies Program at ORNL and is joint faculty at the University of Tennessee's Min H. Kao Department of Electrical Engineering and Computer Science and Bredesen Center for Interdisciplinary Research and Graduate Education.

His group's power electronics research achieved the world's first 120-kilowatt wireless charging system for passenger cars by developing a unique architecture that includes all-ORNL-built power conversion, resonant network and coupling systems. Another focus of Ozpineci's research is the development of lightweight, compact, durable and efficient electric drive system components to improve electric, hybrid and fuel cell vehicles.—*Bill Cabage*

Neutrons open a world of research

by Leo Williams
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If you take a material and place it in a beam of neutrons—one of two particles in the nucleus of an atom—you can get information that is unavailable any other way. Neutrons allow scientists to analyze materials that are difficult to see with techniques like X-rays and electron beams, and they're particularly useful for studying phenomena related to lighter elements in the presence of heavier ones.

Neutrons have contributed a great deal to our understanding of the universe and natural phenomena, although we've known about them for less than nine decades. In fact, as late as the beginning of the 20th century, scientists had no real idea what atoms looked like.

The discovery of the neutron, physicists' understanding of how neutrons can be used as a scientific tool, and the establishment of facilities that put that knowledge to use are central to ORNL's history and to the laboratory's identity today.

Neutrons unlock the secrets of matter

The suggestion that the world was made of atoms had been around nearly two and a half millennia, since the time of the Greek philosopher Democritus in the fifth century B.C., but it was pretty much ignored. Plato, in fact, was so unimpressed with Democritus that he wanted the man's books burned.

The idea of the atom sat dormant for more than 2,000 years, until the early 1800s, when English scientist John Dalton for the first time offered up an atomic theory based on experiment and observation. For Dalton, atoms were like hard little balls and were the fundamental building blocks of nature.

His theory sat unchanged for the better part of a century, until English physicist J. J. Thomson discovered the electron in 1897, thereby opening the possibility that atoms were made up of even smaller parts.

Noting that these tiny, negatively charged particles, which Thomson called "corpuscles," had a mass 2,000 times less than that of the lightest atom—hydrogen—and that atoms as a whole had no net electrical charge, either positive or negative, Thompson suggested that atoms comprise clouds of positive charge throughout which the negatively charged electrons are scattered. This was known as the plum pudding model because it reminded people of the bits of fruit scattered throughout that popular English dish.

> *"Neutrons are essential because they can see how atoms move within matter, and they can easily see very light atoms like hydrogen and lithium and sodium that are nearly invisible to other techniques.*
>
> — ORNL Associate Laboratory Director for Neutron Sciences **Paul Langan**

The idea that atoms have a solid nucleus came in 1911 from New Zealand-born physicist Ernest Rutherford, who would eventually be known as the father of nuclear physics. When two of Rutherford's students—including Hans Geiger, co-inventor of the Geiger counter—shot positively charged alpha particles at a thin gold foil, a few deflected off the foil, suggesting that a gold atom has a small, dense center. So much for the plum pudding model.

A few years later, Rutherford showed that the hydrogen nucleus—which we now know is a single proton—was found in the nuclei of other elements. As a result, we can credit him with discovering the proton.

At this point, scientists understood that an atom's nucleus contained protons, which gave the nucleus its positive charge, but it also needed to contain something else to explain why the mass of most atoms is greater than their atomic number—which we now know is equal to the number of protons in the nucleus. The most common explanation was that the nucleus contained both protons and electrons—the two subatomic particles known at the time—with the negatively charged electrons canceling out some of the positive charge of the protons.

It was British physicist James Chadwick—a student of Rutherford's—who determined that the added mass was due to a third atomic particle, which he called a neutron. In 1932, Chadwick announced his findings in a letter to the journal *Nature*, titled "Possible Existence of a Neutron." He followed up a few months later with an article in the *Proceedings of the Royal Society* titled "The Existence of a Neutron."

What makes neutrons special

Neutrons, then, are one of three components of an atom, the others being electrons and protons. (Physicists later discovered that protons and neutrons are made up of even smaller particles called quarks.)

Like all subatomic particles, neutrons follow the laws of quantum mechanics, exhibiting the properties of both particles and waves. Their usefulness depends largely on their wavelengths, which researchers can manipulate by slowing them down to varying degrees. For instance, neutrons with energies characteristic of room-temperature water are known as thermal neutrons and have wavelengths of about 2 angstroms, or close to the distance between atoms.

Neutrons also have magnetic moments, which effectively make them into tiny subatomic magnets. Because of this, neutrons can be used to explore the magnetic properties of materials responsible for technological advances from hard drives to MRI machines.

Neutrons and the bomb

Neutrons can also cause atoms—or technically their nuclei—to split, a process called nuclear fission. That discovery—made by chemists Otto Hahn and Fritz Strassman and confirmed by Lise Meitner and Otto Frisch—took place in a Germany that had already been taken over by the Nazi dictatorship.

The potential for nuclear fission to release massive amounts of energy in a chain reaction soon had scientists looking for ways to develop a weapon of unprecedented power. Chadwick—the neutron's discoverer—joined in the United Kingdom's effort to develop nuclear weapons and, when the U.K. and United States agreed to collaborate on the project, worked with his American counterparts in the Manhattan Project.

Another scientist involved in the Manhattan Project was Ernest Wollan. Wollan was in attendance when the first manmade nuclear reactor—named Chicago Pile-1—went critical below a football field at the University of Chicago in December 1942. He was also on hand when the first continuously operating nuclear reactor went critical the following November in Oak Ridge.

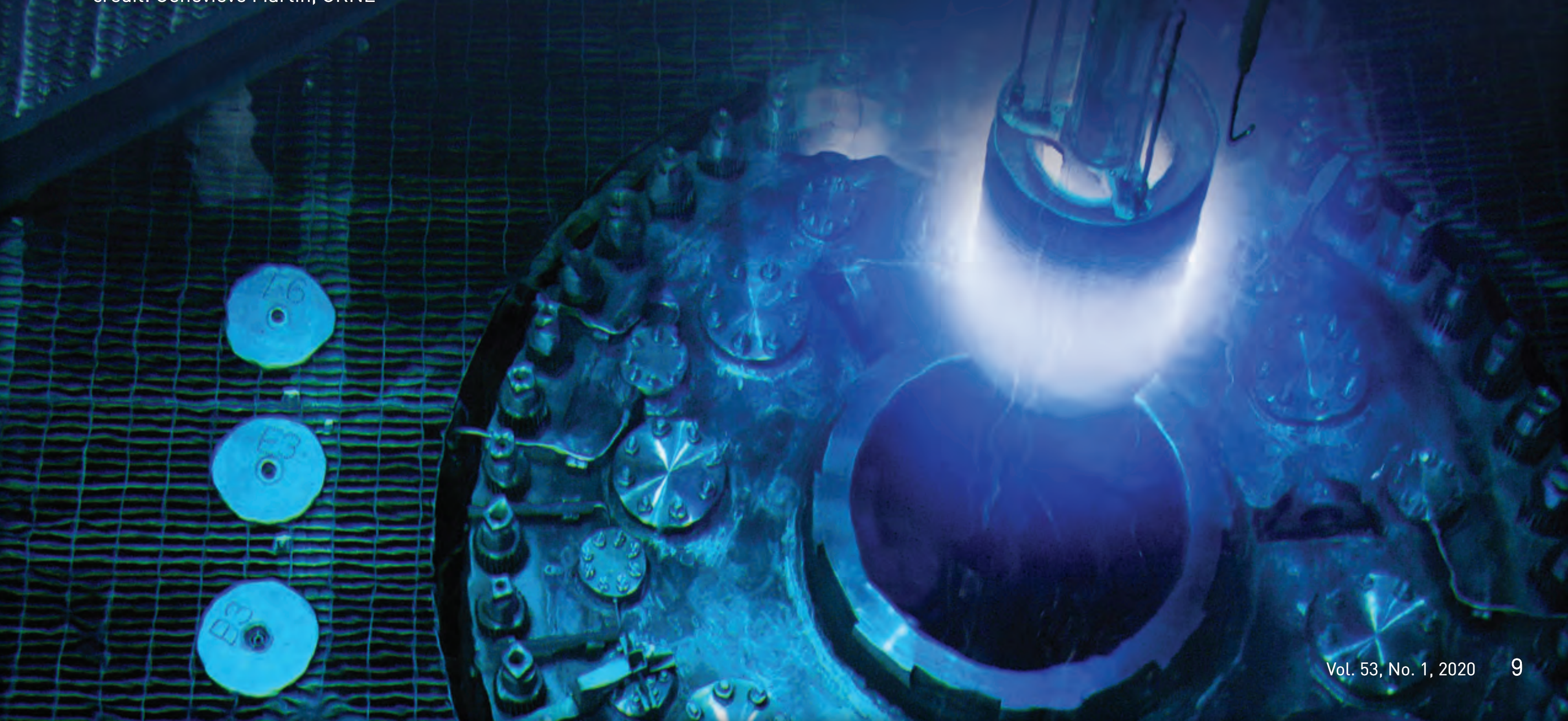
That reactor, located at what would become ORNL, was known at the time as the Clinton Pile and eventually as the X-10 Graphite Reactor.

Neutron science is born at ORNL

Working with the Manhattan Project as a pioneer in the new field of health physics, Wollan measured radiation exposure and developed the film badge dosimeter, but he was also excited by the research possibilities opened up by the new technology (see

See NEUTRONS OPEN A WORLD OF RESEARCH, page 14

ORNL's High Flux Isotope Reactor provides one of the highest rates of continuous-beam neutrons of any research reactor in the world. Image credit: Genevieve Martin, ORNL



What makes

neutron scattering unique

by Leo Williams
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Of the techniques available for studying the structure and dynamics of matter at the smallest scales, neutron scattering is distinguished by the fact that it interacts with an atom's nucleus.

This fact—combined with the fact that neutrons carry no charge—allows researchers to explore matter in ways that are otherwise impossible. In particular, neutrons can analyze materials that contain both light and heavy elements.

Other scattering techniques use photons—which include both visible light and X-rays—and electrons. Because both photons and electrons interact with an atom's electron shell, they are very good at seeing heavy elements, which have a lot of electrons; think of a dental X-ray.

But while photons and electrons scatter off an atom's electron cloud, neutrons penetrate to an atom's nucleus and give you very different information.

"There is a ton of science we do that comes from the unique sensitivity of neutrons to light elements," ORNL physicist Hassina Bilheux said. "If you look at a tissue sample, the X-rays can see the bones, but the neutrons are sensitive to light elements—they see the soft tissue around the bone. That's the complementarity between neutrons and X-rays in imaging."

Because they carry no charge, most neutrons travel through a material without interacting with it. This is both a boon for researchers and a challenge to neutron scattering facilities (see "SNS upgrades will benefit researchers," page 12).

"One of the things with neutrons is they scatter fairly weakly," said Hans Christen, director of ORNL's Neutron Scattering Division. "The majority of the neutrons just go straight through, and most of the neutrons, if they interact once, they will not bounce again. This makes calculations of how neutrons scatter easier than in the case of electrons or photons, which in turn helps to compare measurements to model predictions."

Perhaps an even more important upside to this weak scattering is that neutrons easily penetrate materials that would stop X-rays or electrons, including the containers that must sometimes hold samples. This helps researchers study quantum materials, for example, which must be chilled to temperatures near absolute zero.

> *"There is a ton of science we do that comes from the unique sensitivity of neutrons to light elements. If you look at a tissue sample, the X-rays can see the bones, but the neutrons are sensitive to light elements—they see the soft tissue around the bone. That's the complementarity between neutrons and X-rays in imaging.*
>
> — ORNL physicist **Hassina Bilheux**

The penetrating power of neutrons also allows researchers to look within materials, which is helpful when, for instance, you want to look at a weld without having to cut the metal open.

"We are able to measure averaged strain using neutron radiography," Bilheux said, "which basically tells you how material deforms as you pull or compress it. Using imaging, we are able to give information about the strain through the thickness of the sample. It's pretty neat, because you can start looking at large objects, and it's nondestructive."

ORNL physicist Hassina Bilheux.
Image credit: Genevieve Martin, ORNL

Neutron beams do little damage to cells, proteins, plants and other living systems. Moreover, the sensitivity of neutrons to light elements makes them especially useful for biological explorations. Between ORNL's two neutron scattering facilities—the Spallation Neutron Source and the High Flux Isotope Reactor—a dozen neutron scattering instruments are often used for biology, noted Hugh O'Neill, director of the lab's Center for Structural Molecular Biology.

Looking at magnetism

While neutrons have no charge, they do have magnetic moments—as though each neutron has a tiny bar magnet—which makes them handy for analyzing the magnetic properties of materials, including those responsible for such valuable technologies as computer hard drives and MRI machines. Scientists refer to the magnetic properties of neutrons as their spin.

"Neutrons are sensitive to magnetism," said Matt Tucker, leader of ORNL's Diffraction Group, "so they can be used to determine the magnetic structure as well as the atomic structure. Often the details are not the same, and knowing those differences can tell you about fundamental physics, but also about useful properties of the material."

Neutrons' magnetic properties also make them valuable for studying quantum materials, which are showing promise in areas such as quantum computing, quantum encryption and advanced sensors.

"When a neutron scatters off of a quantum material, the spin of the neutron is going to interact with the magnetic spins in the material," ORNL neutron scattering scientist Clarina dela Cruz said. "We then measure the change in the spin of the scattered neutrons to deduce the nature of the magnetism in the quantum material. This makes neutrons a critically powerful tool in studying quantum materials, as much of their interesting and useful properties stem from the magnetism in them."

See WHAT MAKES NEUTRON SCATTERING UNIQUE, page 15

SNS upgrades

will benefit researchers

by Leo Williams
williamsjl2@ornl.gov

A fundamental understanding of materials is key to solving a broad array of scientific and technological problems. Neutron scattering is a vital tool in building this understanding, and ORNL facilities are critical to keeping the United States at the vanguard of materials research.

ORNL promotes neutron research with two world-class facilities. One, the High Flux Isotope Reactor, produces neutrons continuously by splitting atoms. HFIR has one of the highest neutron fluxes of any reactor in the world, with flux referring to how many neutrons pass through a given area in a specific amount of time.

The other, the Spallation Neutron Source, uses a particle accelerator to shoot high-energy protons at a mercury target in pulses, causing neutrons to be knocked loose from the nuclei of the heavy metal atoms.

More power, new target station

Although SNS is already one of the world's most intense sources of pulsed neutron beams for research, a major upgrade is under way. An upgrade of the facility's proton accelerator will double its power, and construction of a second target station will add new research capabilities.

The first upgrade will make it possible to produce more neutrons by taking the facility's proton accelerator from 1.4 to 2.8 megawatts. The project could be completed as early as 2024.

"The more power we have, the more neutrons we can produce and the brighter our neutron beams," said Paul Langan, ORNL's associate laboratory director for neutron sciences. "And as we increase the brightness of our neutron beams, we can do more complex experiments. We can do experiments quicker, and we can do experiments using much smaller samples, which is important for looking at new materials that can only be synthesized in small quantities."

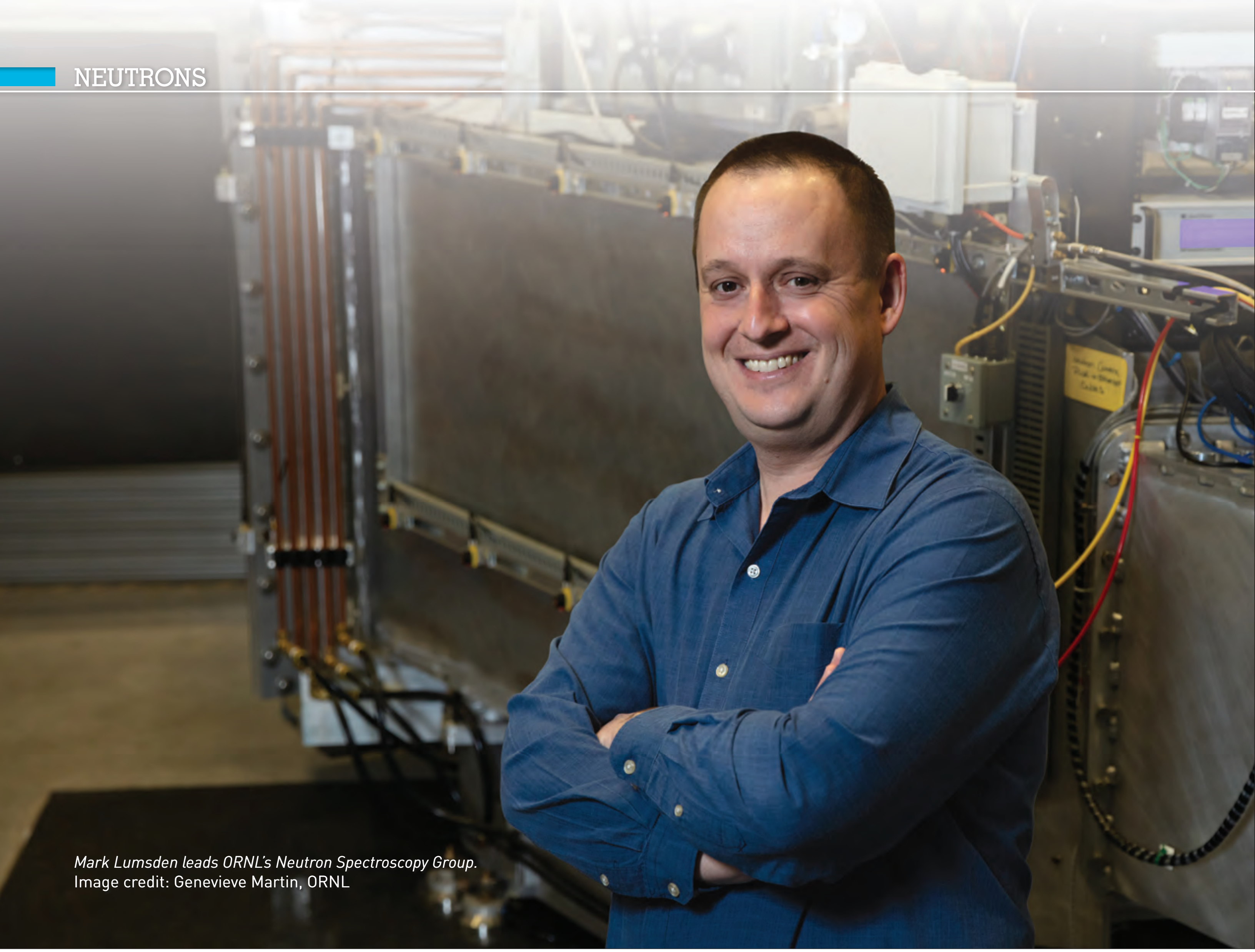
A wider range of neutrons

The second project is to create a new SNS target station geared to a different class of experiments. One key design element of the new target station focuses on the rate at which neutron pulses are delivered. The SNS accelerator produces 60 proton pulses a second, a number that will not change with the power upgrade. The second target station, however, will receive a quarter of those pulses, or 15 a second, with the remainder going to the first target station.

Because there will be a longer interval between neutron pulses at the second target station, researchers will be able to work with a wider range of neutron wavelengths and therefore analyze a wider range of length scales—from an atomic scale counted in tenths of nanometers to a mesoscopic scale that ranges from tens to thousands of nanometers.

"The first target station is optimized for high-precision measurements with thermal neutrons, which are ideal for probing atomic-length-scale phenomena, which tend to be relevant for solid-state materials," explained ORNL physicist Ken Herwig. "The second target station is optimized to produce cold neutrons with longer wavelengths that are optimal for probing behavior at larger length scales. These length scales tend to be more relevant for soft, biological and complex materials."

The second target station could be completed as early as 2028, Langan said.



Mark Lumsden leads ORNL's Neutron Spectroscopy Group.
Image credit: Genevieve Martin, ORNL

NEUTRONS OPEN A WORLD OF RESEARCH, page 9

"What makes neutron scattering unique," page 10). Wollan had a background in X-ray physics, and he wanted to use neutrons in a similar way to unlock the structure of materials.

In May 1944, he asked for and was granted permission to use neutrons produced by the reactor to study the diffraction of neutrons in a single crystal. Using an X-ray diffractometer brought from the University of Chicago and retrofitted at the X-10 Graphite Reactor to become the world's first neutron scattering instrument, Wollan and chemist Lyle Benjamin Borst used neutron diffraction to study crystals of gypsum and sodium chloride, producing a plot known as a "rocking curve."

Their work drew the attention of physicist Clifford Shull, who joined Wollan at Oak Ridge in 1946. The two developed neutron diffraction methods for determining the atomic structure of materials.

Within the next decade, Wollan and Shull worked out how neutrons interact with elements and their isotopes and measured scattering patterns from a wide range of materials. Their achievements included the first neutron radiograph, the first direct evidence of antiferromagnetism (in which the magnetic moments of neighboring atoms point in opposite directions), and the first use of neutrons to determine the structure of hydrogen-containing compounds.

For their pioneering work, Shull received a share of the 1994 Nobel Prize in Physics. Wollan, unfortunately, would not share in that prize because he died in 1984.

Neutron sources beyond the Graphite Reactor

ORNL continued its neutron research in 1958 with construction of the Oak Ridge Research Reactor, which produced beams of neutrons 100 times as intense as those created by the Graphite Reactor.

Then, in 1965, the lab's High Flux Isotope Reactor went into operation. HFIR's primary purpose was to produce radioactive isotopes for medicine, research and industry, but ORNL Director Alvin Weinberg ensured it would continue the lab's work in neutron research, insisting that four beam tubes be installed to transport neutrons from the reactor's core for use in more advanced scattering experiments.

See NEUTRONS OPEN A WORLD OF RESEARCH, page 16

WHAT MAKES NEUTRON SCATTERING UNIQUE, page 11

How we make and use neutrons

Neutron scattering involves creating a beam of neutrons, passing that beam through a sample, and noting where (and possibly when) neutrons scattered from the sample hit a detector. At SNS, a particle accelerator sends protons to collide with a heavy metal target to produce the neutrons in a process known as spallation. At HFIR, neutrons are produced by a nuclear reactor.

Researchers can glean a wide range of information from neutron scattering—how atoms are arranged, for instance, how they're held together, how they're moving around, or which way their own tiny magnets are pointing. Neutrons can zoom in to examine material properties at the atomic scale or, at the other extreme, give you a picture of something as large as a machined part or a living plant.

This impressive range of research depends on the nature both of the neutrons and of the equipment used to study them.

Neutron energy

Neutrons must be slowed substantially before they interact with matter in a way that is useful to researchers. This is done through a process called moderation, in which the high-energy neutrons bounce around in a vessel typically containing hydrogen.

If water—whose molecules contain two atoms of hydrogen and one of oxygen—is used as the moderator, the emitted neutrons have energies that are characteristic of room temperature. These are called thermal neutrons, and their wavelengths are useful for analyzing the atomic structure of a material.

"A thermal neutron has a wavelength that peaks at about 1.8 angstroms, with an angstrom being characteristic of the distance between atoms in a crystalline solid," explained ORNL physicist Ken Herwig. "Having a wavelength of about that distance means that thermal neutrons are sensitive to atomic length scales."

To probe the longer length scales characteristic of proteins, polymers and other "soft" materials, neutrons with longer wavelengths are needed. These "cold" neutrons are created using moderators at much lower temperatures. Cold moderators at SNS are liquid-hydrogen-cooled to about 20 kelvin—or minus 423° Fahrenheit.

Elastic versus inelastic

To obtain a variety of information from neutrons, scientists rely on specialized instruments, with 18 instruments currently residing at SNS and 13 at HFIR. While they explore different aspects of matter, the techniques can be divided into categories such as elastic and inelastic scattering.

In elastic scattering, neutrons bounce off samples without their energy changing. In inelastic scattering, on the other hand, researchers monitor the energy lost or gained by the neutrons.

"In elastic scattering, it's a bit like bouncing Ping-Pong balls," explained Christen. "The scattered particles don't lose any of their kinetic energy, but from the way they scatter, we can determine where the atoms are in the material."

> *"With inelastic neutron scattering, the neutron loses or gains some energy by its interaction with the material. By studying the neutron energy change, we can understand the energy of the interactions between atoms or spins in a material.*
>
> — Neutron Spectroscopy Group Leader
> Mark Lumsden

Neutron diffraction

Neutron diffraction—the technique used to determine a material's structure —mainly uses elastic scattering.

"To determine a material's atomic structure, we shine a beam of neutrons through the material and use a physics equation called Bragg's law," Tucker said. "This law basically says that if there are planes of atoms inside the material, when we shine neutrons at a material, they will bounce off these atomic planes and come out in very specific directions depending on how those atoms are arranged and with a specific brightness depending on the types of atoms present in that plane."

"That will tell us where each particular atom type is located, and then we relate that atomic structure to the properties of the material. Is it a strong material? Is it a weak material? Could it potentially make a good battery material?"

At ORNL, neutron diffraction has been used in a wide range of research, helping researchers search for more reliable cladding for nuclear fuel, better catalysts for producing fuels, and materials for safer and longer-lasting batteries.

Neutron spectroscopy

Neutron spectroscopy takes advantage of inelastic scattering.

"With inelastic neutron scattering, the neutron loses or gains some energy by its interaction with the material," said Mark Lumsden, leader of ORNL's Neutron Spectroscopy

See WHAT MAKES NEUTRON SCATTERING UNIQUE, page 17

Timmy Ramirez-Cuesta leads ORNL's Spectroscopy Team.
Image credit: Genevieve Martin, ORNL

NEUTRONS OPEN A WORLD OF RESEARCH, page 14

HFIR has been going strong for 50-plus years, with no end in sight. Along the way, it has provided important insights into materials such as high-temperature superconductors, rare earth metals and graphite, and has allowed researchers to explore many biological and technological systems.

Adding an accelerator-based neutron source

While nuclear reactors are an important source of neutrons, they are not the only one. Particle accelerators can also be used to produce neutrons, by slamming charged particles into heavy metal targets. This process—known as spallation—is the basis for ORNL's Spallation Neutron Source, which was completed in 2006.

SNS and HFIR make ORNL a destination for neutron researchers worldwide. SNS provides the world's most intense pulsed neutron beams, while HFIR provides one of the highest rates of continuous-beam neutrons of any research reactor in the world.

Between them, they provide powerful tools for analyzing materials, giving researchers the ability to study magnetic behavior, living systems such as cells and plants, and compounds containing both light and heavy elements.

"Neutrons are essential because they can see how atoms move within matter," explained Paul Langan, ORNL's associate laboratory director for neutron sciences, "and they can easily see very light atoms like hydrogen and lithium and sodium that are nearly invisible to other techniques."

Neutron scattering: The next generation

Researchers need intense neutron beams to carry out their experiments. The more powerful the beam, the more information can be gleaned from it.

While SNS is already a world leader in neutron scattering, plans are under way to take it to the next level. These plans include both an upgrade to the facility's accelerator, making it more powerful, and a new target station focused on providing longer-wavelength neutrons (see "SNS upgrades will benefit researchers," page 12).

The power upgrade will take the accelerator from 1.4 to 2.8 megawatts, thereby providing more neutrons and enabling more experiments with smaller samples.

See NEUTRONS OPEN A WORLD OF RESEARCH, page 17

WHAT MAKES NEUTRON SCATTERING UNIQUE, page 15

Group. "By studying the neutron energy change, we can understand the energy of the interactions between atoms or spins in a material."

"Spectroscopy looks more at what atoms do than where they are," said Timmy Ramirez-Cuesta, leader of the Spectroscopy Team. "In particular, in chemical spectroscopy, most of the work looks at how the hydrogen atoms move—how the hydrogen atoms and hydrogen molecules interact with matter."

Neutron spectroscopy can be used to analyze biomaterials or soft materials such as polymers, Lumsden noted. It is also useful in studying thermoelectric materials and quantum materials.

Neutron imaging

A third application of neutrons is neutron imaging—possibly the most easily understood technique. In essence, researchers are making radiographs using neutrons instead of visible light.

Neutron imaging typically looks at scales 100,000 or more times larger than neutron diffraction, Bilheux said—tens to hundreds of micrometers rather than tenths of a nanometer. The technique is useful for research into everything from battery efficiency to water uptake in plant roots.

For example, researchers can put a lithium-ion battery in a neutron beam and examine how well the lithium moves between the battery's anode and cathode over time. The ultimate goal is to develop batteries that last longer and charge faster.

Neutron imaging can also analyze how root systems absorb and manage water under different environmental conditions. In fact, researchers can put living plants in a neutron beam without damaging the plant.

"You can put a root system in the soil, put a pulse of water at the bottom of your can, and see how the roots are taking up water from the surrounding soil," Bilheux said. "The advantage of putting a plant in the neutron beam is we don't damage it."

Neutrons help when "you want to know how to improve crop efficiency in an environment that becomes warmer, or you want to know how plants adapt to drought conditions and what is the proper watering procedure."

NEUTRONS OPEN A WORLD OF RESEARCH, page 16

"The proton power upgrade will make some experiments faster on the first target station," said ORNL physicist Ken Herwig. "It'll mean that we can look at somewhat smaller samples more readily than we could before and do harder experiments. And having more neutrons means measurements that we can do today can be made more quickly, letting us observe changes in samples with better time resolution."

It also means that SNS can add a Second Target Station that provides a wider range of neutrons and is optimized to produce "cold" neutrons with longer wavelengths. By providing that wider range of neutrons, the new target station will allow researchers to examine materials at different scales, from the atomic up 10,000-fold to the mesoscopic scale.

"The First Target Station still will be the neutron source of choice for looking at the structure of materials with atomic resolution or fast dynamics in materials," Langan said. "The Second Target Station will be the source for looking at very complex materials when excellent resolution is needed over a wide range of length or time scales. The High Flux Isotope Reactor still will be the source for looking at materials when detailed measurements in a specific narrow range of length or time scales are required.

"So all three sources are best matched for looking at different scientific problems, and together they really cover everything. It will be unparalleled capabilities for U.S. researchers."

Farewell, Titan:

A long-running supercomputer with tremendous impact

by Katie Jones
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ORNL's Titan supercomputer was decommissioned last August and disassembled for recycling. Its space at the Oak Ridge Leadership Computing Facility is being retrofitted for ORNL's first exascale supercomputer, Frontier, which is slated for delivery in 2021 and will be capable of quintillion calculations a second.

Performing up to 27 quadrillion calculations per second, Titan ranked as one of the world's top 10 fastest supercomputers from its debut as No. 1 in 2012 until June 2019. In its time, Titan served hundreds of research teams around the world working on urgent scientific challenges, providing, for instance, unprecedented simulations of polymers and enzymes critical to the production of cellulosic ethanol, physics-based earthquake hazard models for Southern California and particle-scale plasma simulations for future fusion reactors.

ORNL and OLCF staff said their good-byes to Titan as they gathered in the data center to film HPC systems administrator Don Maxwell shutting down the machine for the last time in August 2019. In the video, the high-pitched whir of Titan's nearly 300,000 CPU cores and 18,688 GPUs fades to silence. ORNL Lab Director Thomas Zacharia shared through social media: "Very proud of the tremendous impact supercomputer Titan has had on the scientific community."

In the weeks following Titan's shutdown, electricians safely disconnected the 9 megawatt-capacity system, and staff from manufacturer Cray disassembled and recycled Titan's electronics and metal components and cabinets.

> *"The reality is, in electronic years, Titan is ancient. Think of what a cell phone was like 7 years ago compared to the cell phones available today. Technology advances rapidly, including supercomputers.*
>
> — Operations Manager **Stephen McNally**

"The reality is, in electronic years, Titan is ancient," said Operations Manager Stephen McNally in summer 2019. "Think of what a cell phone was like seven years ago compared to the cell phones available today. Technology advances rapidly, including supercomputers. ...

"People ask why we can't split up Titan and donate sets of cabinets to different research groups, but the answer is that it's simply not worth the cost to a data center or university of powering and cooling even fragments of Titan. Titan's value lies in the system as a whole."

A new generation of supercomputer

When planning for Titan began in 2009, the high-performance computing community had just the year before passed the petascale barrier, achieving more than a quadrillion calculations per second on two DOE supercomputers: Roadrunner at Los Alamos National Laboratory and Jaguar at ORNL.

However, science never sleeps, and the OLCF was already planning its next supercomputer. This second-generation petascale system would need to be about 10 times more powerful than Jaguar—which had been upgraded to a peak speed of 2.6 petaflops—to meet the growing computational needs of researchers working on complex problems in materials science, biology, physics and other research domains.

Even more challenging than increasing speed, the OLCF's next supercomputer would need to meet DOE goals for cost and energy efficiency, meaning it would need to do 10 times the work while consuming roughly the same amount of energy.

Enter Titan, a new generation of supercomputer with a revolutionary architecture that combined 16-core central processing

Stephen McNally kept Titan running for hundreds of users as National Center for Computational Sciences operations manager. Image credit: Carlos Jones, ORNL

units, or CPUs, and NVIDIA Kepler accelerated processors known as graphics processing units, or GPUs.

The GPUs tackled computationally intensive math problems while the CPUs efficiently directed tasks. When the system debuted at No. 1 in 2012, Titan delivered 10 times the performance of Jaguar with a peak performance of 27 petaflops.

"Choosing a GPU-accelerated system was considered a risky choice," OLCF Program Director Buddy Bland said. "A DOE independent project review committee insisted that we demonstrate that our users would be able to effectively use Titan for the broad range of modeling and simulation applications we support."

Many former Titan users are now solving big science problems on Summit, the OLCF's second GPU-accelerated system that was launched in 2018 as the world's smartest and fastest supercomputer—but Titan will not be forgotten for its revolutionary contributions to computational science.

Igniting a new class of combustion research

by Katie Jones
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The internal combustion engine has been around since the 19th century and remains the most affordable, reliable way to power the American transportation sector and provide electrical power on demand.

But 21st century engines are getting a boost from today's top supercomputers. Through modeling and simulation, scientists and engineers can study how small-scale chemical reactions and turbulence affect performance. By understanding exactly when, where and how fuel burns in the interior of an engine, researchers can improve engine designs and fuel blends to increase efficiency and reduce pollutant emissions.

Over the past five years, researchers led by Jacqueline Chen of Sandia National Laboratories modeled a range of combustion scenarios on the Titan supercomputer at ORNL.

"We need to understand the dynamics of turbulence-chemistry interactions to develop predictive computer models that engine designers can use," Chen said.

Chen's simulations, which use a direct numerical simulation code called S3D to resolve microscale physics, are providing benchmarks that complement experiments for combustion model development and validation.

Once the fastest supercomputer in the world—capable of 27 million billion calculations a second, or 27 petaflops—Titan was decommissioned in 2019, but its impact on research will continue for some time.

Whereas gasoline engines use spark ignition to trigger combustion, diesel engines use autoignition in which pistons compress the fuel-air mixture to high temperatures and pressures until the mixture self-combusts.

Diesel engines are more fuel-efficient than gasoline engines and release fewer greenhouse gases. However, they release more nitrogen oxides and soot and typically come with a higher price tag.

> *"With Titan, we've been able to increase the realism in the actual coupling between turbulent mixing and chemical kinetics associated with ignition for surrogate diesel and gasoline fuels.*
>
> — Sandia National Laboratories researcher **Jacqueline Chen**

"With Titan, we've been able to increase the realism in the actual coupling between turbulent mixing and chemical kinetics associated with ignition for surrogate diesel and gasoline fuels," Chen said.

Cool flames

Accounting for over 20 percent of U.S. petroleum consumption, primarily powering heavy trucks, ships and industrial machines, diesel may be overlooked by millions of passenger car drivers. However, features of the diesel engine are critical to advanced combustion.

In diesel combustion, lower-temperature "cool" flames (less than 1,000 degrees Kelvin, or 1,340 degrees Fahrenheit) ignite and burn, creating the combustible environment for subsequent high-temperature ignition regions.

Researchers estimate that low-temperature combustion could improve diesel engine efficiency by 20 percent. However, unlike spark ignition engines, autoignition in diesel engines is less

controlled, and researchers need to understand the stages of the ignition process.

"We can't resolve these cool flames with sufficient accuracy in physical experiments," Chen said. "The cool flames are extraordinarily thin—that is, a few microns—and the spatial resolution of measurements that can be performed in operating engines is limited."

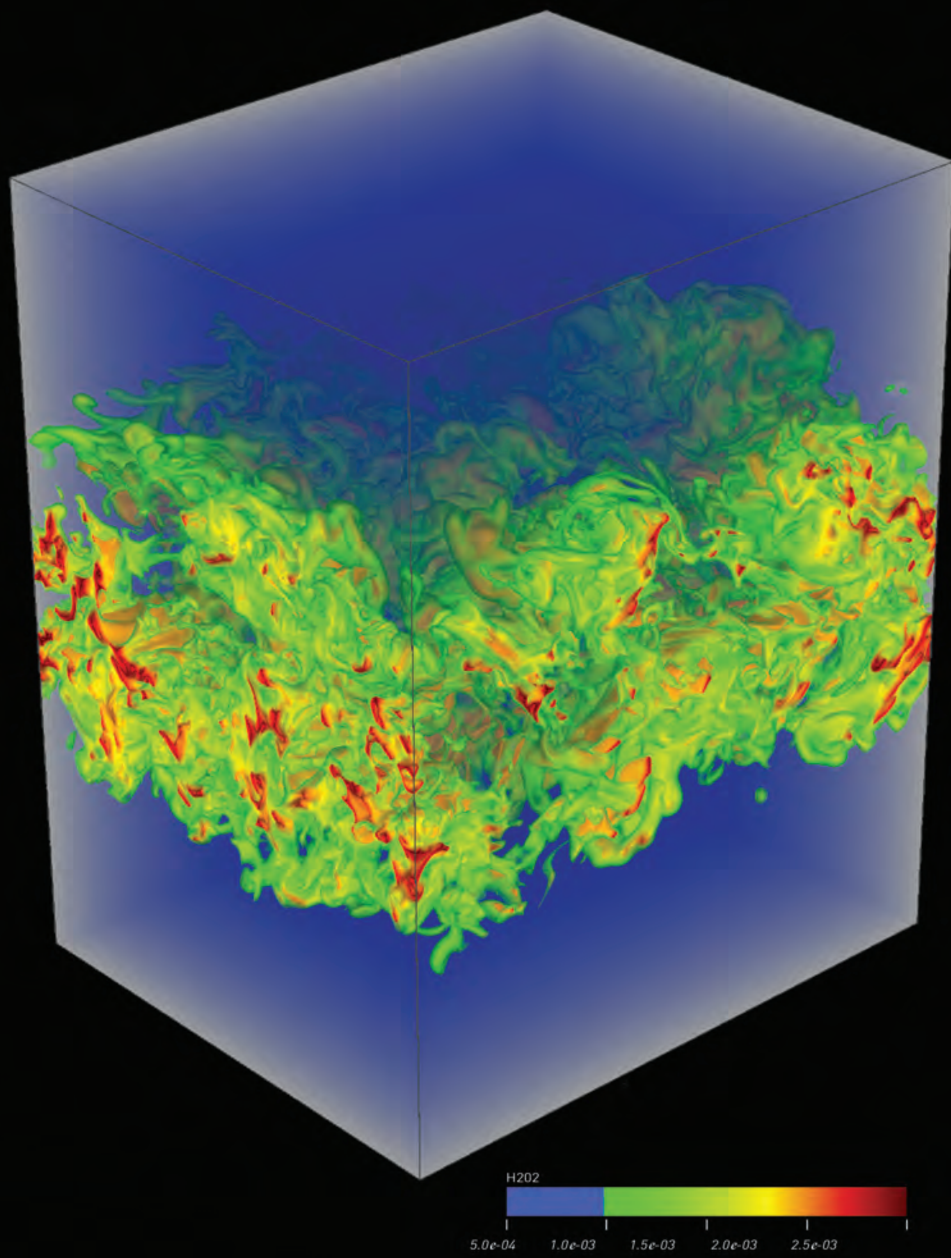
A 2018 journal article authored by Giulio Borghesi of Sandia and coauthored by Chen describes how the team analyzed autoignition under highly turbulent diesel engine conditions requiring 3 billion grid cells at 3 micron resolution and 4 nanosecond time steps using *n*-dodecane as a surrogate for diesel fuel.

The simulations established that low-temperature combustion occurs first, then ignites high-temperature combustion through rapid chemical reactions and heat release coupled with molecular and turbulent transport. Surprisingly, the simulations showed that ignition occurs faster and in more fuel-rich regions than predicted from baseline simulations that do not include transport processes.

With a clearer picture of multistage autoignition, researchers can start to think about optimizing fuel stratification for both ignition timing and flame propagation rates, Chen said.

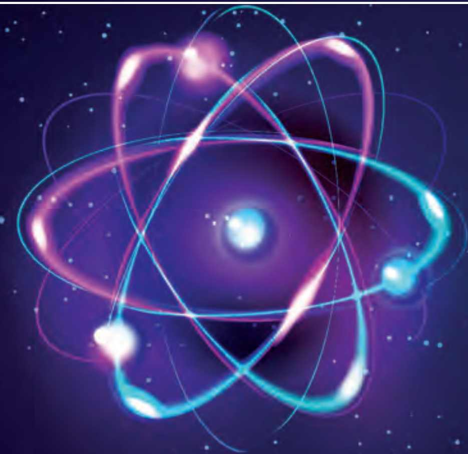
Looking to the future, Chen's team and Tarek Echekki from North Carolina State University will use Titan's successor, the 200-petaflop Summit supercomputer at ORNL, to model more complicated engine geometries, intense turbulent features or complex fuels.

"We're moving up to much higher pressures and finer grid counts and pushing into more realistic regimes," Chen said.



Hydrogen peroxide species undergoing two-stage autoignition in a temporally evolving air/n-dodecane jet. Image credit: Jacqueline Chen, Sandia National Laboratories

Neutron scattering at ORNL



Discovered in 1932, neutrons are one of two particle types found within the nucleus of an atom (the other being protons). Neutrons and protons each consist of three quarks held together by the strong nuclear force.

Why neutrons matter

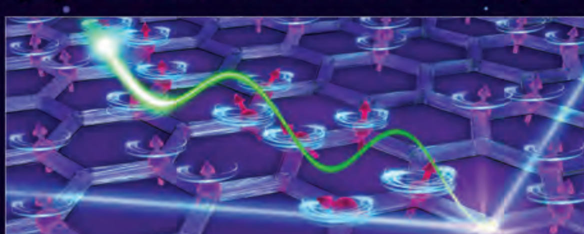
They are uniquely sensitive to light elements such as hydrogen and lithium

- Half the atoms in proteins are hydrogen
- Most catalytic reactions involve hydrogen
- Lithium-ion batteries rely on lithium

They penetrate more deeply than X-rays and electrons

- Neutrons can see through solid containers, making them valuable when samples are liquid or must be kept in extreme conditions
- Neutrons can see inside structures without destroying them

Neutrons have magnetic moments, making them valuable for studying the materials used in electronics and computers

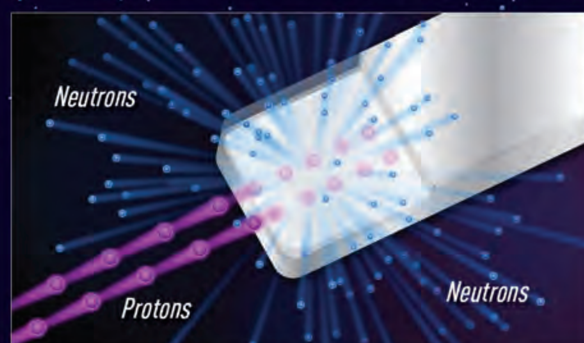


How we produce neutrons

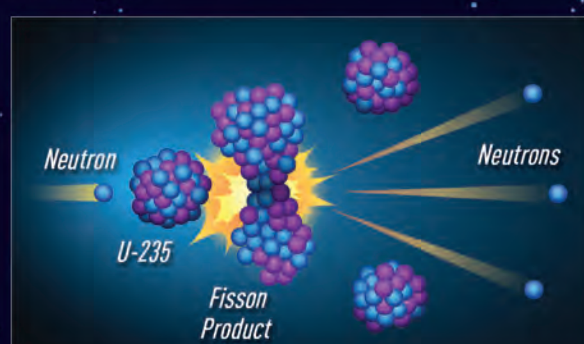
Spallation Neutron Source. The SNS accelerates charged hydrogen ions (with two electrons and one proton) to about 90 percent the speed of light. The ions pass through a foil that removes the electrons and circle an accumulator ring.

The protons are released 60 times a second to smash into a target made of liquid mercury, knocking off neutrons that are then routed to instruments.

When the facility's Second Target Station is completed, protons will be released 15 times a second to strike a rotating tungsten target.

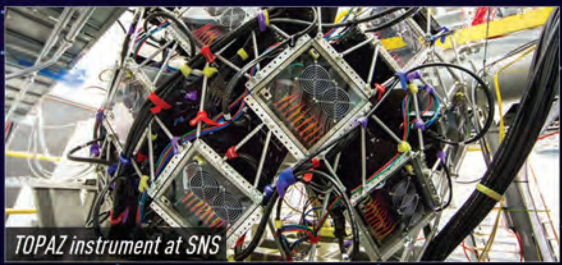


High Flux Isotope Reactor. HFIR is a nuclear reactor that produces neutrons by splitting atoms of uranium-235, with some neutrons splitting other atoms and other neutrons being used to bombard targets.



Types of instruments

Diffraction. Uses neutrons to determine the atomic structure of a material, or where the atoms are in a sample and how they are arranged.



TOPAZ instrument at SNS

Spectroscopy. Uses neutrons to determine the atomic and magnetic motions of atoms.

HYSPEC instrument at SNS

Large structures. Neutron imaging and small-angle neutron scattering instruments study groups of atoms from around 10 nanometers to a micron, including proteins, polymers, and magnetic structures.

Bio-SANS instrument at HFIR

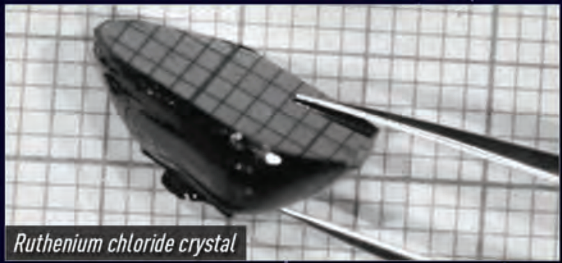
Engineering/imaging. A suite of instruments that use multiple techniques to study the integrity or strength of materials used in industrial applications.

HB-2B beamline at HFIR

New knowledge

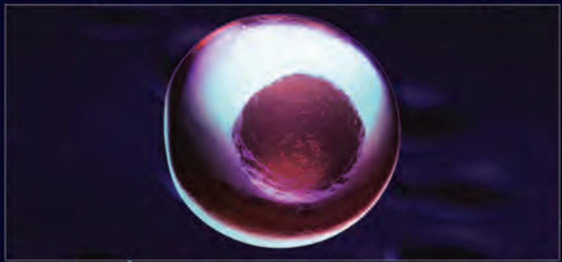
Energy storage. Neutron diffraction is guiding new energy storage technologies by revealing the movement and storage of small electrical charge-carrying ions in materials.

Quantum materials. Neutron spectroscopy is providing new insights into the exotic magnetic behavior of promising materials used in quantum technology.



Ruthenium chloride crystal

Living cells. Neutrons provided the first-ever direct nanoscale examination of a living cell membrane, resolving a long-standing debate by identifying tiny groupings of lipid molecules that are likely key to the cell's functioning.



Better welds. Neutron diffraction allows the Army to test newly developed weld wire for armored vehicles.

Getting to the root of better plants

by Stephanie Seay
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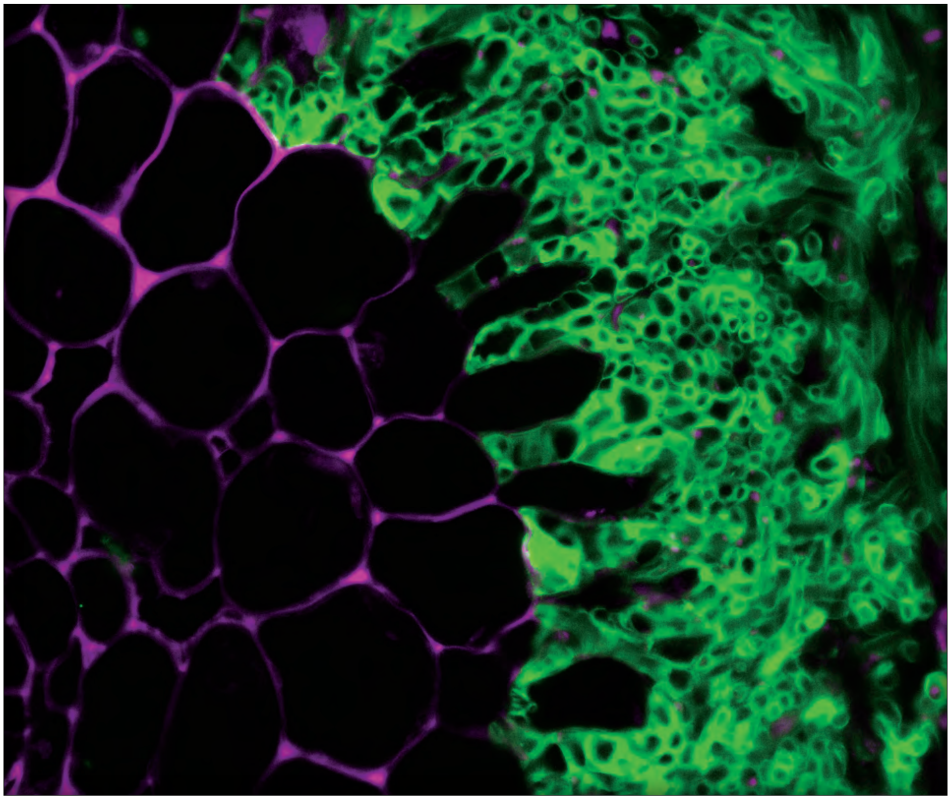
In the production of biofuels from nonfood crops, it helps to start with the right plants. They need to be hardy and grow fast, thriving even in conditions not typically suited for agriculture.

In the search for suitable plants for biofuels production, ORNL scientists noticed that successful candidates had something in common: They had all formed a mutually beneficial relationship with soil fungi.

When united, certain fungi form a protective sheath around plant roots with remarkable benefits, increasing nutrient uptake and even extending outward to communicate with other plants about spreading pathogens and pests. In return, plants feed carbon to the fungal partner, encouraging its growth.



The fungus Laccaria bicolor*, in green, is shown colonizing the root of a natural host* Populus trichocarpa. *A better understanding of plant-fungi symbioses could lead to engineering plant-fungal associations and improve nitrogen and nutrition uptake along with plants' resistance to drought and pathogens.* Image credit: Jesse Labbe, ORNL, and Keven Cope, University of Wisconsin, Madison

More than 80 percent of plant species are able to benefit from this symbiosis. The relationship is believed to have led to the successful colonization of land by plants, enabling vast forests and prairies.

Now, after years of experimentation aided by recent advances in plant genomics and high-performance computing, a team of scientists led by ORNL under the Plant Microbe Interfaces Project has found one of the genetic triggers for the symbiosis and successfully facilitated the relationship in a plant that had been resistant to it.

"We can use this symbiosis to enhance certain conditions in plants such as resistance to drought, pathogens, improving nitrogen and nutrition uptake and more," said ORNL molecular geneticist Jessy Labbe. "The resulting plants would grow larger and need less water and fertilizer, for instance."

The scientists were studying the symbiosis formed by certain species of *Populus*—or poplar trees—and the fungus *Laccaria bicolor* (*L. bicolor*). They used ORNL supercomputers and genome sequences produced at the DOE Joint Genome Institute to narrow down the search to a particular receptor protein, PtLecRLK1. Once they had identified the likely candidate gene, the researchers took to the lab to validate their findings.

They chose to experiment on *Arabidopsis*, a mustard plant commonly used as a model when studying crops, which traditionally does not interact with the fungus *L. bicolor* and even considers it a threat. The

Laccaria bicolor *is fruiting above ground and colonizing the* Populus deltoides *plant root system below ground in a greenhouse setting.* Image credit: Annegret Kohler, INRA-Grand Est, France

scientists created an engineered version of the plant that expresses the PtLecRLK1 protein and then inoculated the plants with the fungus. The fungus *L. bicolor* completely enveloped the plant's root tips, forming a fungal sheath indicative of symbiote formation.

"If we can make *Arabidopsis* interact with this fungus, then we believe we can make other biofuel crops like switchgrass, or food crops like corn, also interact and confer the exact same benefit," said ORNL quantitative geneticist Wellington Muchero. "It opens up all sorts of opportunities in diverse plant systems. Surprisingly, one gene is all you need."

> *"This is a remarkable achievement. Using this technology, we could target as many as 20 to 40 million acres of marginal land with hardy crops that need less water, while supporting rural economies and supplying sustainable alternatives for gasoline and industrial feedstocks.*
>
> — ORNL Center for Bioenergy Innovation Director **Jerry Tuskan**

The work dovetails with one of the key goals of the Center for Bioenergy Innovation at ORNL: to create sustainable biomass feedstock crops. "This is a remarkable achievement," said CBI Director Jerry Tuskan. "Using this technology, we could target as many as 20 to 40 million acres of marginal land with hardy crops that need less water, while supporting rural economies and supplying sustainable alternatives for gasoline and industrial feedstocks."

The scientists plan to continue analyzing the engineered symbiosis and to conduct similar experiments with plants such as switchgrass and rice.

ORNL engine research

supports new fuel development

by Jennifer Burke
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When ExxonMobil was searching for a research partner to operate a one-of-a-kind experimental engine that would enable the development of next-generation lubricants for the marine industry, one place topped the international oil and gas company's list: ORNL.

Custom-built to one-tenth scale by Mahle Powertrain and Seacoast, the flexible-fuel, single-cylinder marine diesel engine, called the Enterprise, stands 12 feet tall and weighs more than 16,000 pounds, with a rated speed of 625 rpm to match the linear average piston speed of a full-scale engine.

ORNL researchers at the National Transportation Research Center study the impact of lubricants on the marine engine's efficiency and durability. Image credit: Carlos Jones, ORNL

"ExxonMobil came to ORNL because we know fuels and emissions, and we know engines," said Mike Kass, senior engineer and principal investigator on the project. "However, we knew land engines and nothing about this particular unconventional two-stroke marine engine, so we had a learning curve."

> *"We've met all of our objectives with this project. That's because ExxonMobil understands that science is necessary to meet the low-sulfur regulation. They respect the science and research side of it. It's been uncharted territory for both of us, but we've worked through all of this together to achieve our goals.*
>
> — ORNL senior engineer and principal investigator **Mike Kass**

Since the Enterprise was commissioned in 2016 at the DOE's National Transportation Research Center at ORNL, Kass and his team have not only navigated that learning curve, they've also conducted research to inform ExxonMobil products such as a new suite of low-sulfur fuels. Called EMF.5, the suite adheres to sulfur-compliant marine fuel specifications.

"The research at ORNL allowed ExxonMobil to perform controlled engine-based experiments and filled the gap between bench-scale and full-engine tests," Kass said. "This engine has been an integral part of ExxonMobil's whole research strategy to develop next-generation lubricants."

The marine industry is facing the challenge of transitioning to low-sulfur fuels. The International Maritime Organization's low-sulfur fuel requirement begins in 2020, stipulating that container ships must reduce the sulfur content of vessel fuel from 3.5 percent to 0.5 percent. Fuels lower in sulfur produce fewer emissions and therefore reduce air pollutants. ORNL's research exploring the impact of various lubricant formulations on fuel efficiency is expected to lead to new lubricant products that will improve energy efficiency.

"Marine ships are longer than the Empire State Building is tall and wider than a football field," Kass said. "Fuel accounts for 50 percent of operation costs, and the sulfur emissions from one ship equates to 50 million cars. When you think about more than 90 percent of all goods across the world being shipped via cargo vessels, the pressure on the marine industry to comply with this sulfur regulation is tremendous."

At the NTRC, Kass and fellow researchers Eric Nafziger and Brian Kaul continue to collect invaluable data on the Enterprise, running the engine for weeks at a time to determine the impact of lubricants or oils on engine efficiency and durability, including wear and corrosion. The team conducts experiments in controlled environments.

"These controlled-environment experiments allow us to eliminate variables such as weather patterns, cargo loads and temperature that would impact the performance and isolate the effects of

ORNL's marine engine research team, from left, Mike Kass, Eric Nafziger and Brian Kaul, work with ExxonMobil at the National Transportation Research Center. Image credit: Carlos Jones, ORNL

lubricants," Kaul said. "Those things do impact fuel efficiency in the field and make it difficult to get repeatable experimental results. That's an advantage of laboratory experiments here, because we aren't subject to some of those uncontrolled fluctuations that make it difficult to resolve the effects we're looking for."

Kass added that the team is working to install a fuel system to conduct experiments that evaluate the performance of various ExxonMobil lubricants in protecting the engine from wear, corrosion and deposits with new fuel.

As research continues, Kass and his team will continue processing data from the engine, monitoring its performance as it steadily runs at NTRC.

"We've met all of our objectives with this project," Kass said. "That's because ExxonMobil understands that science is necessary to meet the low-sulfur regulation. They respect the science and research side of it. It's been uncharted territory for both of us, but we've worked through all of this together to achieve our goals."

Bio-inspired material soaks up oceans' uranium

by Ashley Huff
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Harvesting uranium from seawater may become more efficient and less expensive, thanks to a low-cost polymer adsorbent developed by researchers from ORNL, Lawrence Berkeley National Laboratory, the University of California at Berkeley and the University of South Florida.

Uranium deposits in seawater are abundant and replenishable because of the natural erosion of ore-containing rocks and soil. Despite relatively low levels—approximately 3 milligrams of uranium per ton of seawater—the world's oceans hold massive stores of the element totaling an estimated 4 billion tons, or about 1,000 times more than all land sources combined.

With a practical recovery method, saltwater extraction would offer a sustainable alternative to uranium mining that could fuel nuclear power production for millennia. The development of efficient uranium adsorbents to harness this potential resource, however, has been an elusive quest since the 1960s.

"Our approach is a significant leap forward," said ORNL chemist Ilja Popovs, who took inspiration from iron-hungry microorganisms to create a new material with a natural affinity for uranium.

Microbes such as bacteria and fungi secrete natural compounds known as siderophores to siphon essential nutrients like iron from their hosts. "We essentially created an artificial siderophore to improve the way materials select and bind uranium," Popovs said.

The team used computational and experimental methods to develop a novel functional group known as H_2BHT that selects uranyl ions, or water-soluble uranium, over competing metal ions from other elements in seawater, such as vanadium.

> *"The goal is to develop efficient adsorbent materials at a low cost that can be processed using mild conditions to recover uranium, and also reused for multiple extraction cycles.*
>
> — ORNL chemist **Alexander Ivanov**

The fundamental discovery is backed by the promising performance of a proof-of-principle H_2BHT polymer adsorbent. Uranyl ions are readily adsorbed, or bonded to the surface of the material's fibers, because of the unique chemistry of H_2BHT.

The prototype stands out among synthetic materials for increasing the storage space for uranium, yielding a highly selective and recyclable material that recovers uranium more efficiently than previous methods.

Selectivity has long been a stumbling block on the road to more efficient adsorbent materials. Early advances, driven by trial and error, found that amidoxime-based functional groups effectively bind uranium in water but do an even better job of recovering vanadium, although the latter has a comparatively lower concentration in seawater.

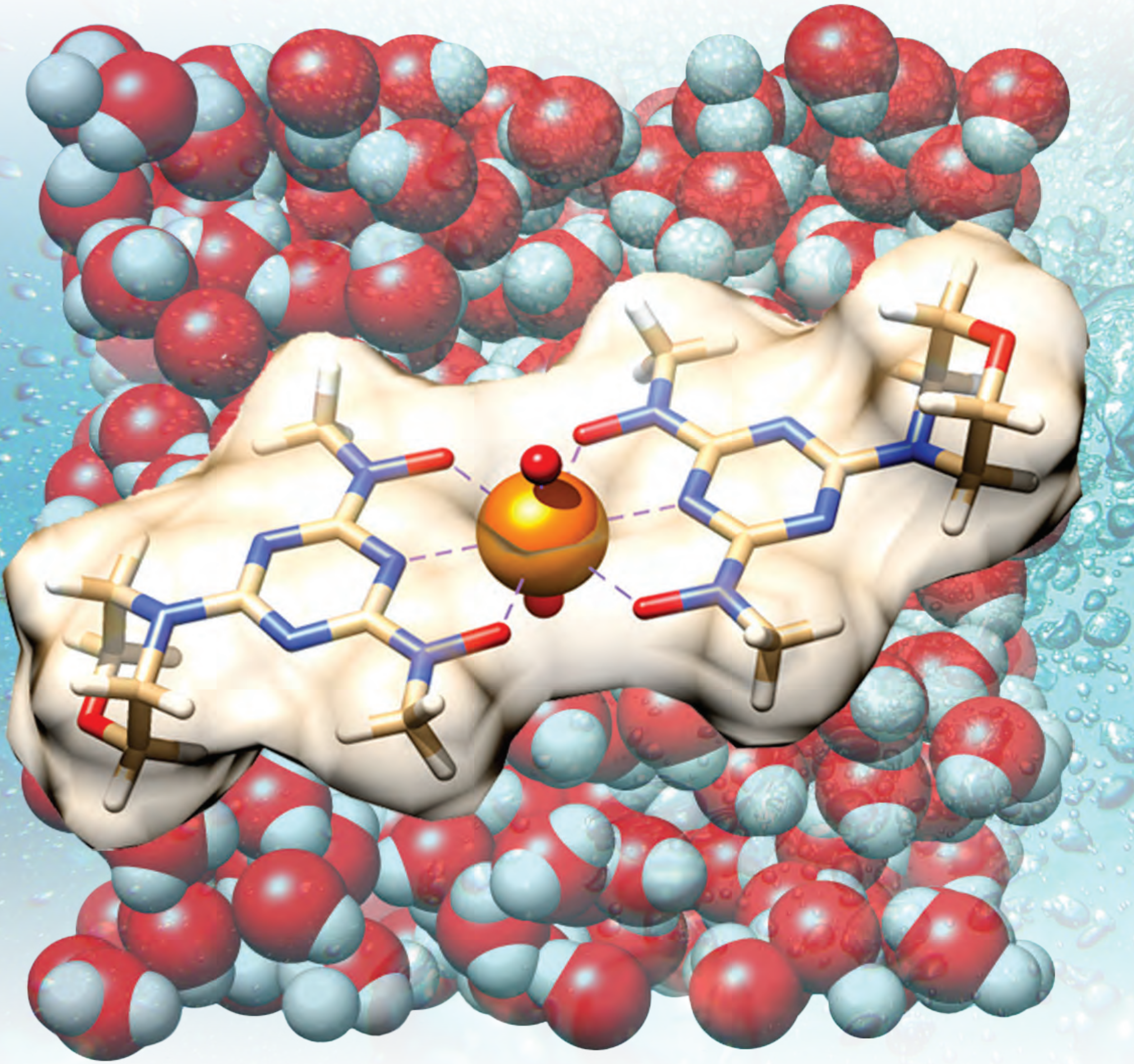
The team previously studied amidoxime-based compounds to investigate their potential, revealing a fundamentally stronger attraction to vanadium than to uranium, which could be a roadblock to progress.

"The result is that amidoxime-based materials, the current front-runners for commercially available adsorbents, fill up more quickly with vanadium than with uranium, which is difficult and costly to remove," Popovs said.

Highly concentrated acidic solutions used to remove vanadium are more expensive than mild or basic processing solutions and are burdened by caustic waste streams. Moreover, acid processing can damage material fibers, which limits their reuse, making commercial adoption cost prohibitive.

"The goal is to develop efficient adsorbent materials at a low cost that can be processed using mild conditions to recover uranium and also reused for multiple extraction cycles," ORNL chemist Alexander Ivanov said.

The team's H_2BHT material offers an alternative approach to better target uranium in mixed-metal water environments.



Researchers combined fundamental chemistry with high-performance computing at ORNL to demonstrate an efficient, low-cost method for recovering uranium from seawater. Image credit: Alexander Ivanov, ORNL

"Our material is tailor-made for selecting uranium over other metals present in seawater and can easily be recycled for reuse, making it much more practical and efficient than previously developed adsorbents," Popovs said.

Unlike vanadium-laden materials, the H_2BHT polymer can be processed using mild basic solutions and recycled for extended reuse. The eco-friendly features also bring significant cost advantages to potential real-world applications.

The next step, say researchers, is to refine the approach for greater efficiency and commercial-scale opportunities.

Right electrolyte

doubles 2D material's ability to store energy

by Dawn Levy
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Scientists at ORNL and Drexel University and their partners have discovered a way to improve the energy density of promising energy-storage materials, conductive two-dimensional ceramics called MXenes.

Today's batteries, which rely on charge stored in the bulk of their electrodes, offer high energy-storage capacity, but slow charging speeds limit their use in consumer electronics and electric vehicles. Tomorrow's energy-storage mainstays may be supercapacitors, which store charge at the surface of their electrode material for fast charging and discharging.

Currently, however, supercapacitors lack the charge-storage capacity, or energy density, of batteries.

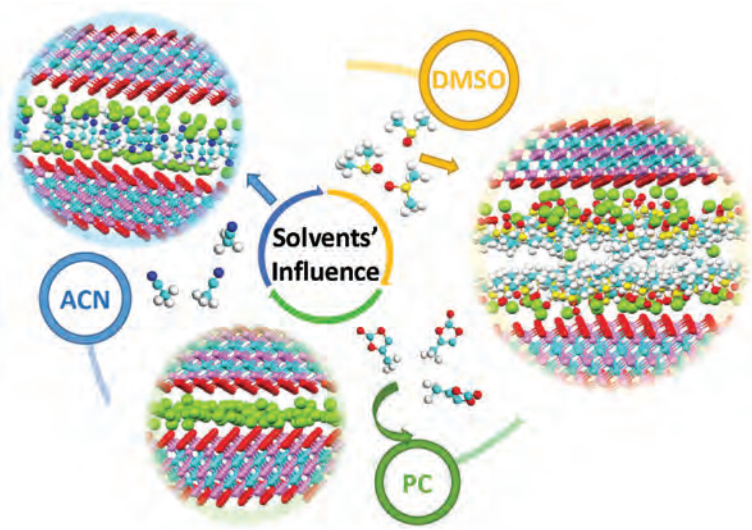
"The energy storage community is conservative, using the same few electrolyte solvents for all supercapacitors," said principal investigator Yury Gogotsi, a Drexel University professor who planned the study with postdoctoral researcher Xuehang Wang. "New electrode materials like MXenes require electrolyte solvents that match their chemistry and properties."

The surfaces of different MXenes can be covered with diverse terminal groups, including oxygen, fluorine or hydroxyl species, which interact strongly and specifically with different solvents and dissolved salts in the electrolyte. A good electrolyte solvent–electrode match may then increase charging speed or boost storage capacity.

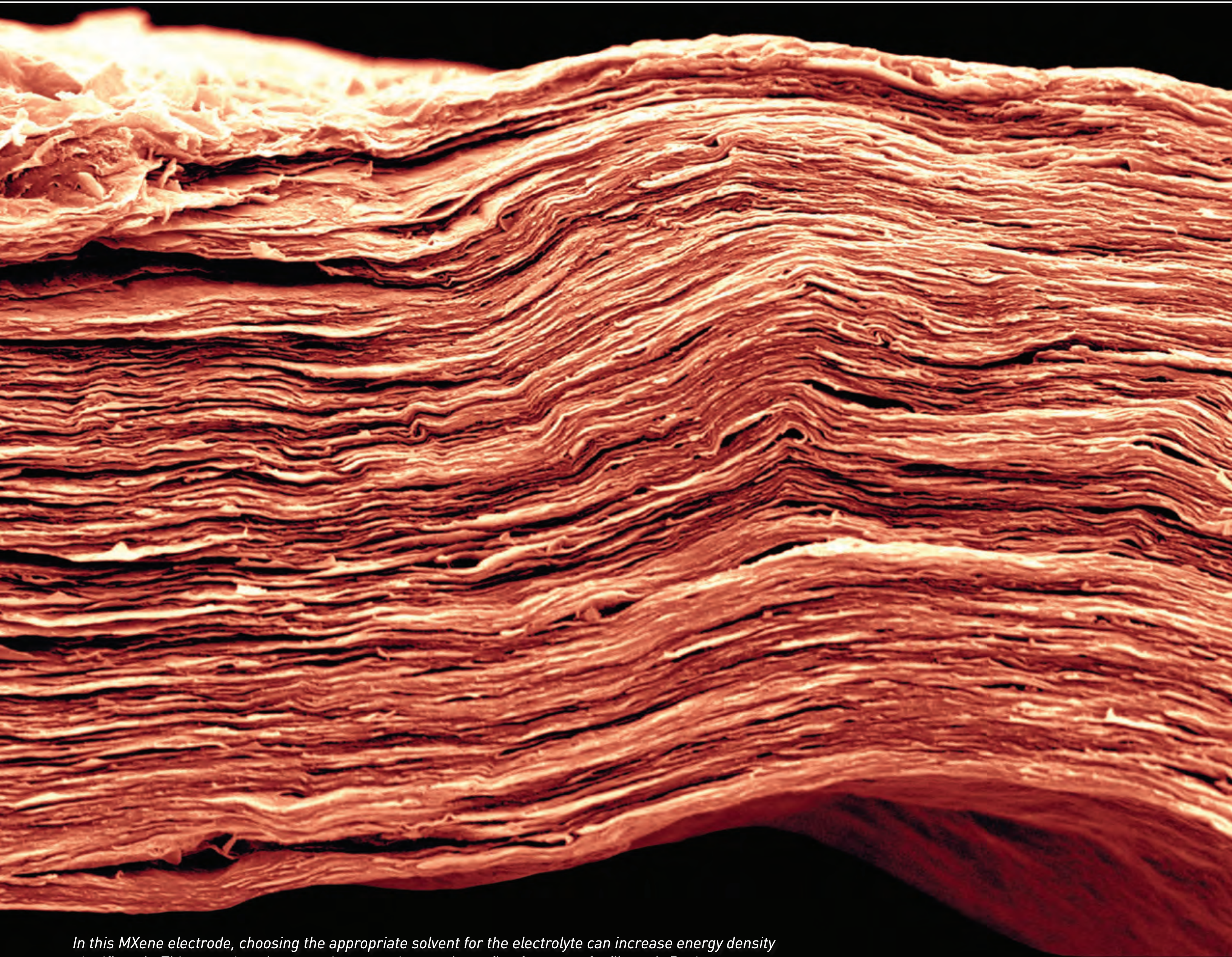
"Our study showed that the energy density of supercapacitors based on two-dimensional MXene materials can be significantly increased by choosing the appropriate solvent for the electrolyte," added coauthor Lukas Vlcek of the University of Tennessee, who conducts research in UT and ORNL's Joint Institute for Computational Sciences. "By simply changing the solvent, we can double the charge storage."

The work was part of the Fluid Interface Reactions, Structures and Transport—or FIRST— Center, an Energy Frontier Research Center led by ORNL and supported by DOE's Office of Science. FIRST research explores fluid–solid interface reactions with consequences for energy transport in everyday applications.

Drexel's Ke Li synthesized the titanium carbide MXene from a ceramic containing titanium, aluminum and carbon by etching



MXene electrodes were soaked in lithium-based electrolytes in three dramatically different solvents (acetonitrile, ACN; dimethyl sulfoxide, DMSO; and propylene carbonate, PC). The PC solvent produced the highest energy density because lithium ions were "naked" (not surrounded by solvent), allowing the tightest packing of positive charges between MXene layers. Image credit: Xuehang Wang, Drexel University, and Lukas Vlcek, ORNL



In this MXene electrode, choosing the appropriate solvent for the electrolyte can increase energy density significantly. This scanning electron microscopy image shows fine features of a film only 5 microns thick—approximately 10 times thinner than a human hair. Image credit: Tyler Mathis, Drexel University

out the aluminum layers to form five-ply MXene monolayers of titanium carbide.

The researchers then soaked the MXenes in lithium-based electrolytes in various solvents with different structures and properties. The electrical charge was carried by lithium ions that easily insert themselves between MXene layers.

Electrochemical measurements showed that the maximum capacitance (amount of energy stored) was achieved using a less conductive electrolyte, based on a propylene carbonate solvent. This was unusual: a commonly used acetonitrile solvent–based electrolyte would be expected to deliver the best performance.

In situ X-ray diffraction showed expansion and contraction of the MXene interlayer spacing during charging and discharging when acetonitrile was used, but not when the propylene carbonate solvent was used. The latter solvent resulted in much higher capacitance. Furthermore, electrodes that don't expand when ions enter and exit are expected to survive a larger number of charge-discharge cycles.

To probe the dynamics of electrolyte solvent media confined in the MXene layers, the researchers turned to neutron scattering, which is sensitive to hydrogen atoms contained in the solvent molecules.

Finally, molecular dynamics simulations done by Vlcek revealed that interactions among the lithium ions, electrolyte solvents and MXene surfaces strongly depend on the size, molecular shape and polarity of the solvent molecules. In the case of a propylene carbonate–based electrolyte, the lithium ions are not surrounded by solvent and therefore pack tightly between MXene sheets. However, in other electrolytes, lithium ions carry solvent molecules along with them as the lithium ions migrate into the electrode, leading to its expansion upon charging. Modeling may guide the selection of future electrode–electrolyte solvent couples.

The future is bright:

Nine ORNL researchers take home prestigious early career awards

by Abby Bower
ornlreview@ornl.gov

ORNL works hard to attract talented young researchers. Clearly, these efforts have borne fruit, as evidenced by our early career award winners.

In 2019, nine ORNL early career researchers were recognized with prestigious awards from the White House and the Department of Energy—the Presidential Early Career Award for Scientists and Engineers, or PECASE, and the DOE Early Career Research Program Award.

Established in 1996, the PECASE is "the highest honor bestowed by the U.S. government on outstanding scientists and engineers beginning their independent careers and who show exceptional promise for leadership in science and technology."

Winners in 2019 included two from ORNL: David Cullen of the Center for Nanophase Materials Sciences and Kate Page of the Neutron Scattering Division.

DOE Early Career Research Award recipients include seven from ORNL—a lab record and the most of any institution. The Early Career Research Program grants national lab recipients $500,000 annually for five years to cover research expenses and salary, with the award selection based on peer review of research proposals.

ORNL recipients are Leah Broussard of the Physics Division, Miaofang Chi of the Center for Nanophase Materials Sciences, Lucas Lindsay of the Materials Science and Technology Division, Joseph Lukens of the Computational Sciences and Engineering Division, Josh Michener of the Biosciences Division, Catherine Schuman of the Computer Science and Mathematics Division, and Yangyang Wang of the Center for Nanophase Materials Sciences.

"ORNL is proud of our early career researchers," Laboratory Director Thomas Zacharia said. "We seek to attract the very best and to encourage collaboration and creativity. These awards highlight a passion and commitment that will benefit the United States and the world for years to come."

We sat down with these promising young scientists to talk about their backgrounds and current research. Read their profiles on the following pages.

Chasing big physics problems

Leah Broussard

by Abby Bower
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Leah Broussard has always embraced challenges.

"I like to chase problems," she said. "I go wherever I find the most fun."

Chasing problems is what first led her to physics in her early teens, when someone told Broussard that was the hardest thing she could do. It also inspired her Early Career Award-winning proposal, "Systematics of precision neutron physics experiments."

The research will push boundaries in precision by characterizing systematic uncertainties—tricky data errors that arise from inaccuracies in measurement or observation—for two of the world's most ambitious physics experiments, both being conducted at ORNL's Spallation Neutron Source. These are a neutron beta-decay experiment called the "Neutron 'a' 'b'"—or Nab—and the upcoming neutron Electric Dipole Moment, or nEDM, experiment.

The Nab uses neutron decay to explore the weak interaction between quarks—tiny particles that make up protons and neutrons. It will test the Standard Model, which encompasses our understanding of three of the four fundamental forces (the strong and weak forces and electromagnetism).

The nEDM experiment studies neutrons for a small separation of charge called the electric dipole moment. If a large enough EDM is found, it would indicate missing physics in the Standard Model that could explain why the universe contains matter but almost no antimatter, Broussard said. Such findings would help inform a new model—one that solves these unanswered physics questions.

Broussard will seek to improve Nab's precision by measuring timing inaccuracies in the detection of protons and electrons produced during neutron decay. For the nEDM, she'll create more realistic models of the experiment using ORNL's Summit supercomputer to reduce uncertainties caused by false signs of an electric dipole moment.

A project incorporating both Summit and SNS is perfect for Broussard, who triple-majored in math, physics and computer science at Tulane University. She earned a doctorate in physics from Duke and spent three years at Los Alamos National Laboratory before accepting a Wigner Fellowship at ORNL in 2016.

She chose ORNL specifically for the kind of high-level neutron work she's doing now.

"This work can tell us something fundamental about our universe," Broussard said.

Trying to 'see' electrons

Miaofang Chi

by Abby Bower
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Ever since she first encountered microscopes in elementary school, Miaofang Chi has been enchanted by the idea of unlocking worlds invisible to the naked eye.

"To me, it's a kind of artwork," Chi said. A lifelong photography lover, she views microscopy similarly, as a way to capture and share fantastic moments that might otherwise be obscured.

Chi has committed her career to electron microscopy, which uses electron beams to magnify items to degrees unachievable through optical methods. After earning her master's in materials science and engineering from the Shanghai Institute of Ceramics, she studied scanning transmission electron microscopy—or STEM—during her Ph.D. program at the University of California, Davis. She joined ORNL in 2008.

Today's state-of-the-art STEM can observe the atomic makeup of materials and reveal how atoms bond and interact. However, viewing electric fields—necessary for Chi's research on batteries—is still difficult.

Chi sought solutions in a novel technique called STEM-based differential phase contrast, or DPC, imaging, which showed promise in imaging traditionally difficult light elements, like lithium and hydrogen. Successes with the technique inspired her to push it further.

"I said, 'Well, we can see nuclei, even single protons; how about electrons by themselves?'" she explained.

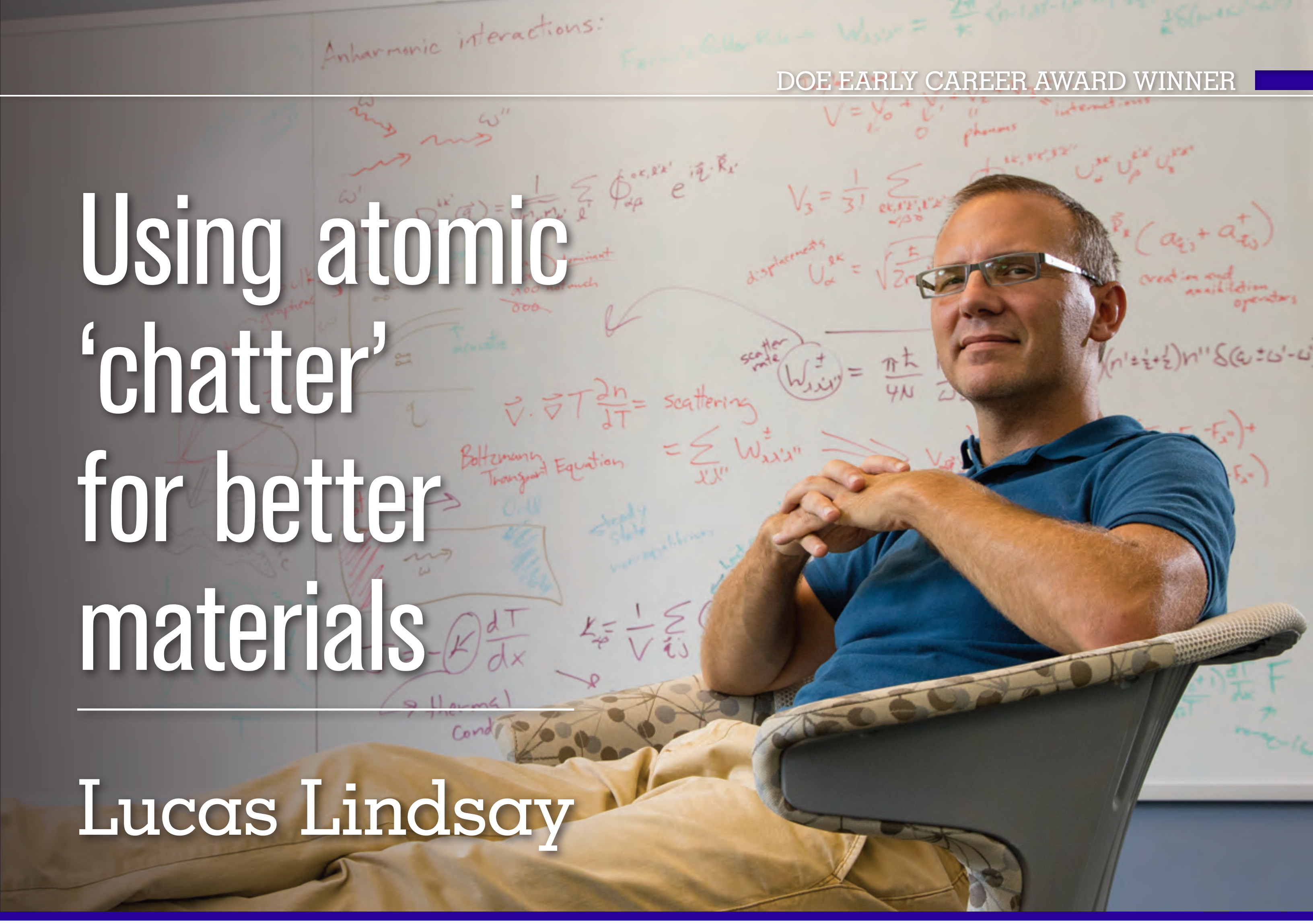
She'll seek to image the subatomic particles, which have never been directly observed through microscopy, for her Early Career Award-winning proposal, "Probing anionic electron behavior in electrides."

In her research, she'll use DPC imaging to "see" electrons in newly discovered materials called "electrides." The materials have unusual structures and localized "free" electrons, unlike typical substances.

"Because of those special electrons, electrides could have really interesting quantum phenomena" that could improve energy technologies and nanoelectronics, Chi said.

The work combines two major themes of her career—advancing innovative microscopy techniques and applying them to new materials.

"As I progressed in microscopy, I started seeing it as a way to understand how materials behave," Chi said. "Then we can design and develop materials for specific applications, which can improve daily life."



Using atomic 'chatter' for better materials

Lucas Lindsay

by Abby Bower
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In his research studying atomic vibrations called phonons and their role in heat flow, Lucas Lindsay searches for materials that are quirky—a word he also uses to describe himself.

"I like looking for things that don't do exactly what you think they should and figuring out why," Lindsay said. "You have to dig in and use these tools you have—the underlying physics—to try to understand the curiosities."

Lindsay's path to computational materials physics wasn't straightforward. After high school, he traveled the United States, returning home to work "dead end" jobs and start a punk band.

He later enrolled at the College of Charleston as an English major. There he tried a philosophy course that led to a chemistry course that led to a physics course.

"It went downhill from there," he joked.

Lindsay earned his Ph.D. in physics from Boston College, where he studied thermal transport in carbon nanotubes and graphene. He came to ORNL in 2014 after teaching college physics and earning a fellowship at the U.S. Naval Research Laboratory.

His Early Career Award-winning proposal, "Elucidating the nature of chiral and topological phonons in materials for energy technologies," will investigate ways to fine-tune materials' thermal conductivity by focusing on the "chirality" of vibrating atoms.

Chirality is a property of certain molecules that occurs when their mirror images don't overlap, in the same way that right and left hands are different, Lindsay says. He's found that this property affects how phonons "talk" to each other. The more phonons talk, or "chatter," with one another, the less heat they can carry.

"I want to use this concept to manipulate phonon scattering and find materials that have high thermal conductivity though we'd think they wouldn't, given other properties," Lindsay said.

"Your phone, your car, your batteries get hot," he adds. Controlling heat is especially important in computing, as more densely packed transistors need efficient materials to carry heat away.

While applications of his research span everyday life, Lindsay enjoys the mysteries involved in his work.

"I love the puzzles," he said. "I think that's what I like about physics."

Building networks of light

Joseph Lukens

by Abby Bower
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Joseph Lukens picked electrical engineering as his undergraduate major at the University of Alabama, thinking it might help him manipulate sound.

"I thought it might help me become an audio engineer or something like that," Lukens said. An avid bass guitar player and history buff, he'd been accepted to music programs but found better engineering scholarships.

Now, four years after earning his Ph.D. in electrical engineering from Purdue University and joining ORNL as a Wigner Fellow, Lukens works to control not sound, but light.

Specifically, he uses single light particles, photons, to "advance our ability to use light for quantum information," he said.

"Quantum information processing could transform how we measure, process and communicate information," Lukens said. It's recognized for its potential to improve data security and solve currently unsolvable computational problems—capabilities owed to unique characteristics.

In classical digital communication, information exists in discrete states of 0 and 1. Quantum information differs because quantum bits, or qubits, can exist as 0 and 1 simultaneously in the fragile state of "superposition." The fact that photons are both waves and particles means that their 0 and 1 states can add together and interfere, like two different waves, even though only one particle is involved. Because these states are so sensitive to disruption, qubits make good sensors and secure data channels.

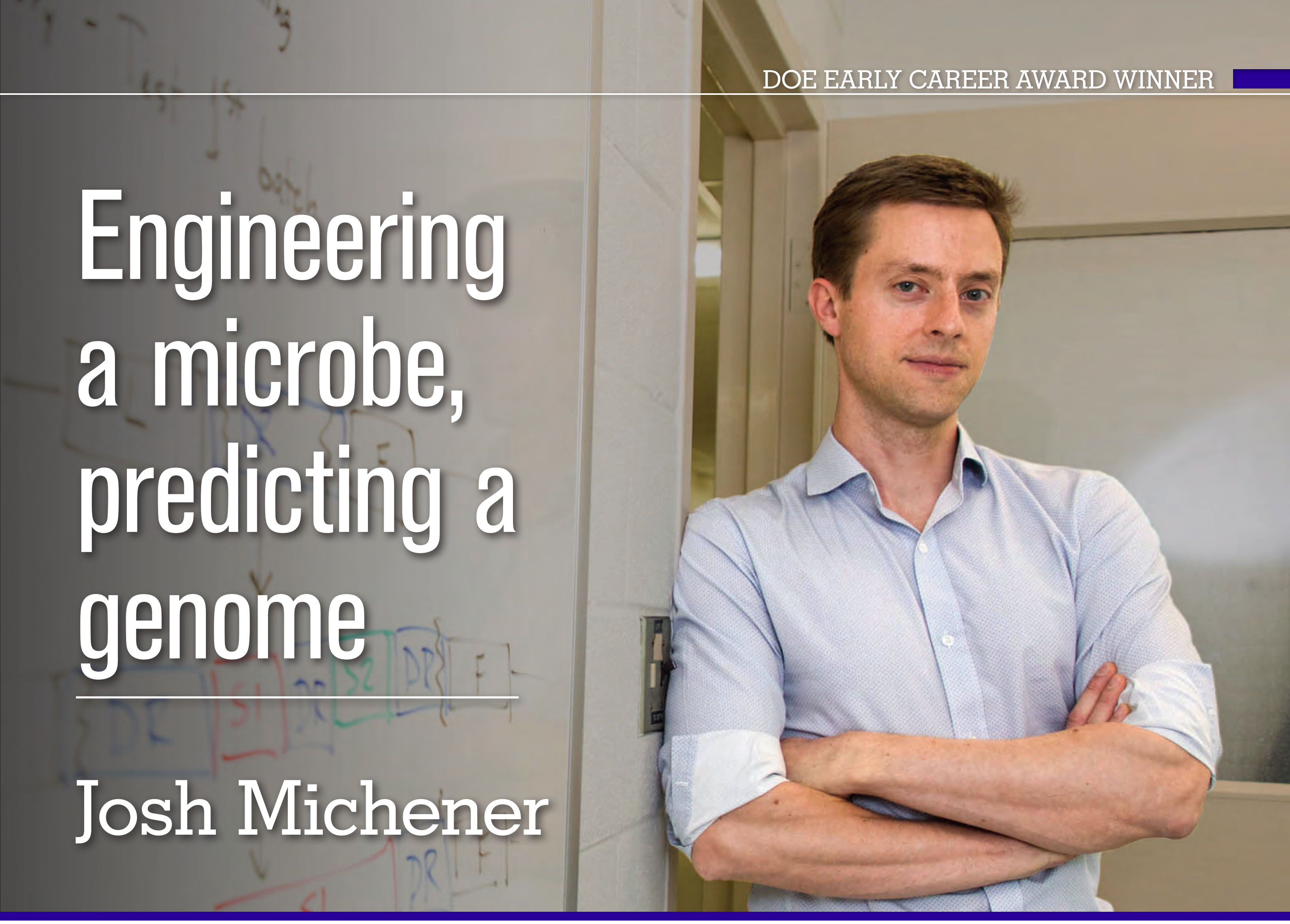
But for building networks, these qualities can cause major problems.

Lukens' Early Career Award-winning proposal, "Scalable architectures for hybrid quantum/classical networking," seeks to overcome some of those barriers.

Using quantum nodes that communicate through the color of light, he'll investigate ways to build networks that support coexistent classical and quantum information—a difficult task, since quantum information is easily destroyed by interference from classical data. He'll also scale up networks and develop "transducers" that can convert information between systems.

It's a big challenge, but that's never bothered Lukens.

"That's how we move science forward," he said. "We have to take risks and work hard to deliver on them. When you're able to figure out solutions, there's no feeling like it in the world."



Engineering a microbe, predicting a genome

Josh Michener

by Abby Bower
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When biological engineers try to genetically modify an organism, they often don't know what most of the organism's genes actually do.

Josh Michener wants to change that.

"I'm an engineer," Michener said. "I want to be able to write a design and go make it. We don't understand biology well enough to do that."

Michener knew by high school that he wanted to pursue a career in science, but when asked which field he'd pick, his stock answer was, "I don't know, but not biology." That changed during his undergraduate years studying chemical engineering at the Massachusetts Institute of Technology.

"The parts of chemical engineering that most interested me were really biochemical engineering," he said. "Then, as I got deeper into bioengineering, I realized I should learn more of the biology."

Michener earned his Ph.D. in bioengineering from Caltech and followed it with a postdoctoral fellowship in evolutionary biology at Harvard. He joined ORNL as a Wigner Fellow in 2015.

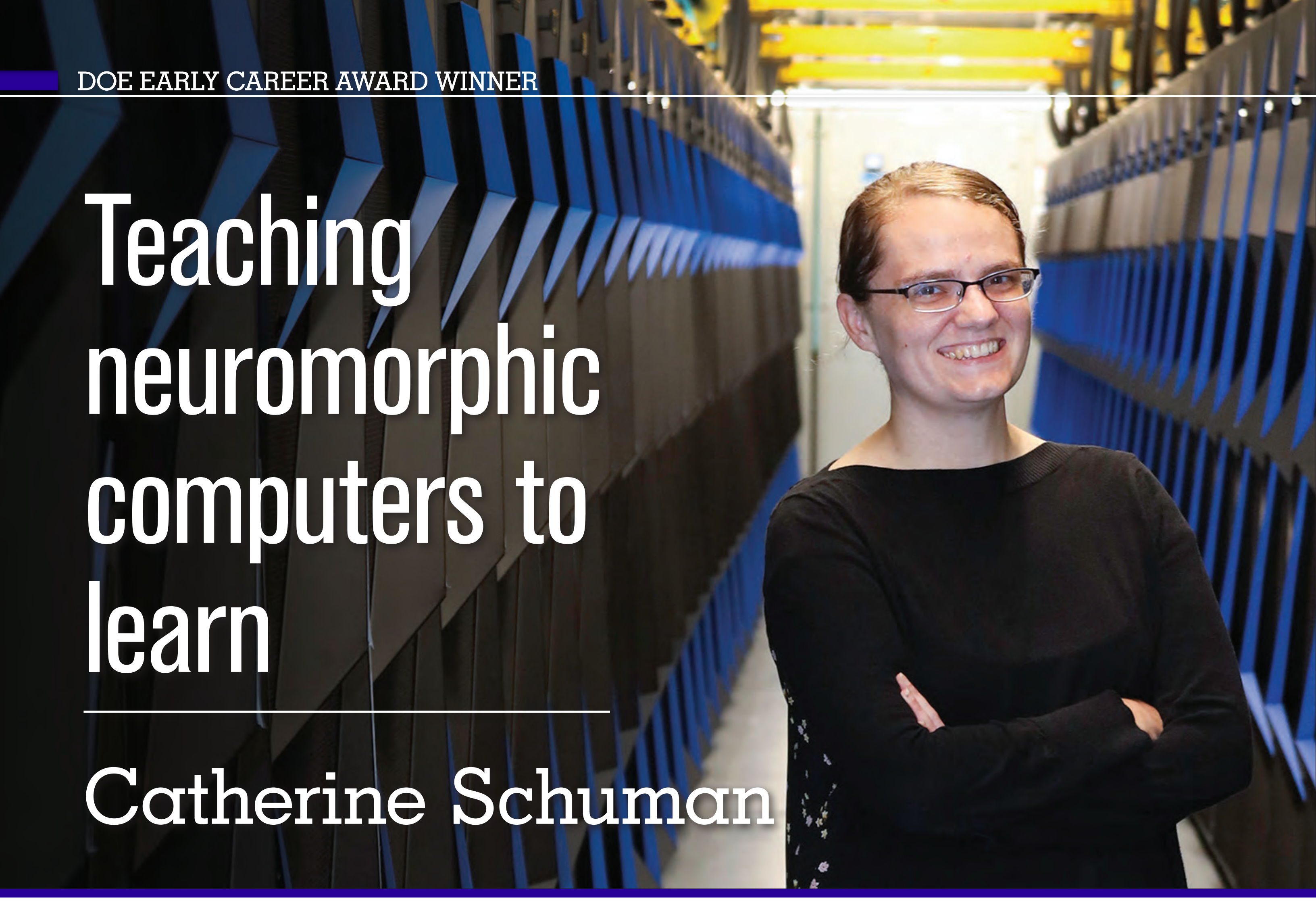
His Early Career Award-winning proposal, "Systems metabolic engineering of *Novosphingobium aromaticivorans* for lignin valorization," will examine one microbe's capacity to break down lignin—a stubborn polymer that acts as the structural "glue" in woody plants but also becomes a low-value byproduct of biorefineries. Finding higher-value uses could help make biofuels more economically viable.

Michener will build a "parts list" of desirable genes that help *N. aromaticivorans* degrade lignin. To do that, he'll use a novel genetic method to create a computational model that can predict effects of mutations throughout an organism's genome.

The method, which Michener and his team developed at ORNL, involves randomly swapping alleles—or alternative forms of a gene—and testing their physical expressions, or phenotypic effects, he said.

He'll also scale up his experiments, aiming to test around 100 times more strains in a single experiment than would be possible using traditional methods, which will provide ample data to build the predictive computational system he finds so exciting.

"It's exciting to go from 'crazy idea' to 'it's actually working, and we can make discoveries with it,'" Michener said. "We have the chance to discover some new biology, some new engineering tools, and to learn to be better biological engineers."



Teaching neuromorphic computers to learn

Catherine Schuman

by Abby Bower
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Even as a child, Catherine Schuman liked the challenges fundamental to computer science.

"I always liked puzzles, especially analytical puzzles," Schuman said. "Code is exactly that."

Her father, a math teacher, and her brother, a programmer, introduced Schuman to computers early, but as a teenager, the Harriman, Tennessee, native also enjoyed biology. She kept a pamphlet detailing the mammalian genetics research at ORNL's "Mouse House" on her bookshelf.

Today, her research on neuromorphic computing—a novel, energy-efficient technology that mimics biological neural networks like those in the human brain—allows Schuman to combine both interests. The speed, efficiency and localized networks of neuromorphic computers make them useful for a wide range of applications, from autonomous vehicle sensing to edge computing, in which data is stored and processed near where it is generated.

Schuman became interested in nature-inspired machine learning techniques such as neural networks as an undergraduate studying computer science and math at the University of Tennessee, where she stayed for her Ph.D. in computer science. At ORNL in 2015, she accepted a Liane B. Russell Fellowship—named after the pioneering geneticist whose work inspired Schuman years earlier.

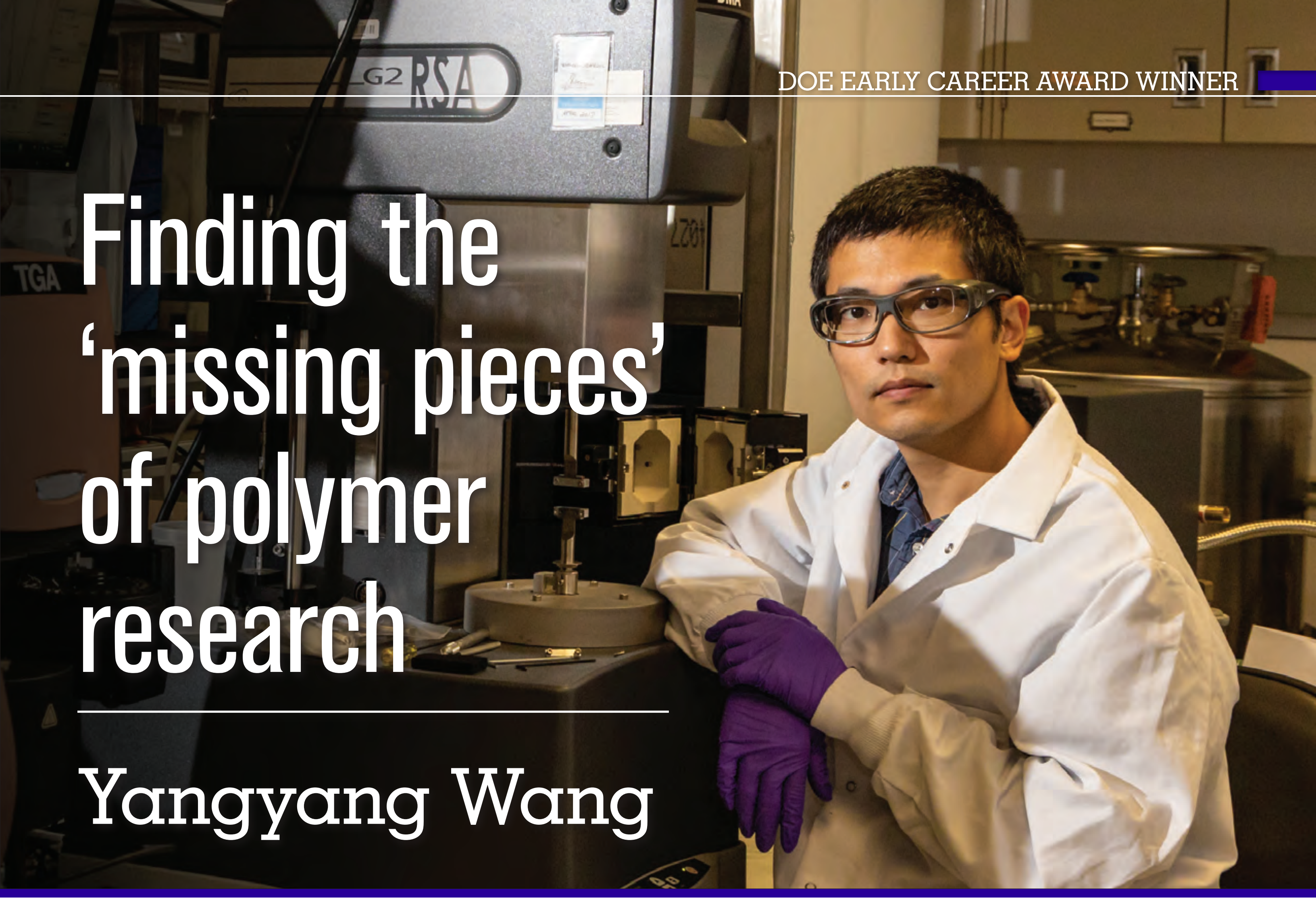
For her Early Career Award-winning proposal, "Learning to learn: Designing novel neuromorphic algorithms with machine learning," Schuman will use machine learning with high-performance computing to develop new training and learning algorithms for neuromorphic computers. Algorithms are instructions computers follow to solve problems.

The first step in the research is to simulate neuromorphic hardware, which swaps traditional processing systems for artificial neurons and synapses, on ORNL's Summit and upcoming Frontier supercomputers. She'll imitate what neuromorphic chips, which are still very new, might look like in the future.

Then, she'll use high-performance computing with the simulators she built to study existing learning algorithms, aiming to improve the algorithms for the new hardware.

Last, she'll use machine learning to develop entirely new algorithms. The goal is to find approaches to analyze scientific data using neuromorphic computers, since the novel systems show promise in overcoming limitations of traditional computing.

"Being able to use the world's fastest computers to explore innovative ways of doing machine learning for new types of computers is really exciting," Schuman said. "You get to do something for the first time, which is not always the case."



Finding the 'missing pieces' of polymer research

Yangyang Wang

by Abby Bower
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Polymers, the focus of Yangyang Wang's research, are all around us.

"We can find them anywhere," Wang said, glancing around his office in the Center for Nanophase Materials Sciences. "In this cell phone, in this plastic bag—everything we use in our daily lives."

He's interested in the diverse applications of the chain-like molecules, but what fascinates him most is using neutrons to find "missing pieces" in our current understanding of how polymers behave as they flow and deform.

Wang found polymer science while pursuing an undergraduate degree in chemistry from Peking University. He earned his Ph.D. from the University of Akron's polymer science program before accepting a postdoctoral position at ORNL. He learned neutron scattering and computer simulation—techniques essential to his current research—after joining the CNMS in 2014.

His Early Career Award-winning proposal, "Fingerprinting macromolecular flow and deformation with neutrons," will explore methods for understanding polymer behavior on the molecular level, starting with small-angle neutron scattering.

"You can imagine it as taking snapshots of a molecule when it deforms and stretches," Wang said. "This technique helps us study how the molecule has changed its conformation."

Using neutron spin-echo spectroscopy, Wang said he'll observe how molecules "change shape in space and time," adding a dynamic element. Mathematical analysis of both methods will help paint a complete picture of the way a polymer behaves under stress, its "dynamic fingerprint." This can improve the ability of manufacturers to produce materials with desirable properties, such as elasticity.

The dynamic fingerprint, Wang explained, is a way to make sense out of a beautiful but otherwise meaningless set of information—a reflection of his evolving relationship to science.

"As a kid, you typically accept what other people tell you, and people tell you science is great," Wang said of growing up in Beijing, where science careers are celebrated. "As you start doing science, it gets more personal. You find meaning in your job. We're paid to create knowledge and learn new things."

PRESIDENTIAL EARLY CAREER AWARD WINNER

Award validates years of work

Kate Page

by Jim Pearce
pearcejw@ornl.gov

PECASE winner Kate Page knows the world of neutron research from the inside out, having worked both as a scientist supporting users at neutron facilities at Oak Ridge and Los Alamos national laboratories and as an accomplished experimentalist in her own right.

"Winning a PECASE award felt like a great validation of the years of working with the user communities and conducting experiments at neutron sources in the U.S.," said Page, formerly of ORNL's Neutron Scattering Division and now an assistant professor in the University of Tennessee's Materials Science and Engineering Department.

"I think I received the award because I have done a lot of work on both of those fronts."

Page's award cites the importance of her work in using "neutron total scattering data" to understand the structure of materials. This technique—which involves studying structure simultaneously on both large and extremely small scales—is helping scientists to understand some of the quirky properties of materials.

"Often what makes materials interesting and work the way they do is in the details of how they are ordered at the very smallest atomic level," Page explained. "Picture a brick wall—from far away it might look pink, but if you're close up, you can see the bricks are gray and red.

"Our technique allows us to see similar distinctions in materials at the atomic level. We tie those differences to material functionalities—like the way a battery charges and discharges or the way a material has resilience against radiation damage. These things are tied to how the materials are ordered at the atomic scale, and we can probe that with this technique."

Page said that while she doesn't think that her PECASE award will change the direction of her research, it reminds her that there's more to scientific endeavor than focusing on your own career.

"I think it just reminded me that as you gain success in your career, it's really important to think about how you can contribute to those around you and those you are interacting with," she said.

Succeeding with world-class collaborators

Dave Cullen

by Jim Pearce
pearcejw@ornl.gov

For having just won a PECASE award, Dave Cullen is a pretty humble guy.

"The award is a big deal, and it's a big honor," he said, "but I think it's a reflection of more than just the individuals; it's a reflection of their institutions and the people surrounding them."

Cullen, an electron microscopist at ORNL's Center for Nanophase Materials Sciences, suggests that his award for research into the factors that control the durability and performance of fuel cell materials owes a great deal to the unique combination of world-class staff, collaborators and facilities at ORNL.

"We have state-of-the-art equipment and the expertise that goes with that," he said. "That's critical to ensuring that your research reaches the level at which it gets noticed for this type of award.

"Also, in my case, collaborations were very important—both inside and outside the lab—through the CNMS and through DOE's Fuel Cell Technology Office and Energy Materials Consortium. Thanks to these relationships, I'm working with top-notch scientists who are doing the best science."

Cullen emphasized the importance of user facilities like CNMS in bringing together innovative researchers from around the world.

"I don't think you'd see these types of opportunities at a university," he said. "Having a nanoscience center means we can bring in external users. That really increases the breadth of our collaborations. We have engagement with fuel-cell researchers who are working in Japan, Asia, Israel and so forth. The CNMS has really enabled international collaboration."

Cullen hopes that the prestige of his PECASE award will help to jump-start new collaborations that will extend the advances he and his colleagues have made in the field of fuel cell research to other energy conversion technologies.

"We are already seeing the techniques we have developed with electron microscopy for fuel cell catalysts extended naturally to other energy conversion systems, including CO_2 conversion," he said. "With the prestige of the award and the attention that comes with it, we now have opportunities to develop other collaborations in new areas that relate well to the technique that we have developed."

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.

Riley Hanus

Postdoc, Materials Science and Technology Division
Ph.D., Materials Science and Engineering, Northwestern University
Hometown: Clear Lake, Iowa

What are you working on at ORNL?

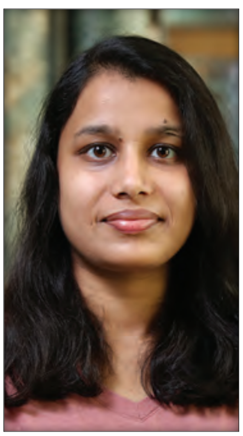
I am performing neutron scattering experiments and theoretical simulations to establish materials design principles for heat conduction in defective and complex crystals. The goal is to provide the basic scientific understanding required to guide the development of next-generation energy technologies, such as power electronics and thermoelectrics.

What would you like to do in your career?

I would like to establish the scientific understanding and technological capability required to improve global quality of life and ensure a sustainable future. More specifically, I aim to apply materials physics in practical ways to advance technology. Where our basic understanding is insufficient, I strive to pave new ground.

Why did you choose a career in science?

I find science challenging, rewarding and quite fun. Additionally, I enjoy the thought that the work I do may someday be impactful and useful in the betterment of society.



Payal Chirania

Graduate student, Chemical Sciences Division
Ph.D. student, Biological Mass Spectrometry, University of Tennessee
Hometown: Kolkata, India

What are you working on at ORNL?

My research focuses on understanding bacterial metabolism for use in bioenergy research. I am using mass spectrometry and bioinformatic methods to explore the mechanisms by which microorganisms break down plant material in natural environments. This knowledge can be applied in industries to enhance biofuel production.

What would you like to do in your career?

I want to continue working in the field of systems biology and explore new data analysis methods, given the amount of data biology is generating. Having a background in both experimental and computational methods, I want to use this experience to better identify solutions in health care and the environment.

Why did you choose a career in science?

Two words—curiosity and creativity—have attracted me to science. I have always been intrigued by the sophisticated mechanisms of the natural environment. Science helps me explore these mechanisms and employ them in innovative ways to our benefit.

Dante Quirinale

Postdoc, Neutron Technologies Division
Ph.D., Condensed Matter Physics, Iowa State University
Hometown: Swanton, Vermont

What are you working on at ORNL?

I develop and use levitators to study materials with neutron scattering at very high temperatures. Topics I'm currently working on include the nature of magnetic ordering in liquid metals, potential prenucleation clustering in industrially important melts, and microscopic understanding of creep deformation at ultra-high temperatures.

What would you like to do in your career?

I hope to keep finding difficult questions that require unique, out-of-the-box solutions—particularly involving ideas that can change our understanding of the liquid state. Ideally, those solutions would help develop the next generation of materials.

Why did you choose a career in science?

I love the feeling of diving deep into a new and exciting problem, especially in a team of like-minded professionals. In physics, those problems often lead to deep rabbit holes and many questions. And there is a chance these questions can push the envelope of what we know is possible.

Pedro Vicente Valdez Jr.

Graduate student, Reactor and Nuclear Systems Division
Ph.D. student, Nuclear Engineering, University of California, Berkeley
Hometown: Tijuana, Mexico

What are you working on at ORNL?

I work on validating the upcoming Molten Salt Reactor modeling capabilities of the SCALE simulation suite. More specifically, I focus on modeling the online fuel processing systems available in MSRs and studying their impact on several reactor physics parameters—like reactivity and poison fraction and their effects on factors like the breeding potential.

What would you like to do in your career?

I would like to contribute to making Generation IV advanced nuclear reactors a reality. The world is in need of clean and sustainable baseload energy, and I truly believe nuclear–renewable hybrid energy systems are the solution. This is why I plan on dedicating my career to advance reactor modeling.

Why did you choose a career in science?

I have always been fascinated with knowing how things work. How does a power plant produce energy? What materials are needed in environments as harsh as a nuclear reactor core? With science, specifically nuclear engineering, I found a way to continue answering many of these intriguing questions while helping the global warming challenge.

Mengya Li

Graduate student, Energy and Transportation Science Division
Ph.D. student, Mechanical Engineering, Vanderbilt University
Hometown: Beijing, China

What are you working on at ORNL?

My research is focused on sodium-ion batteries, primarily on engineering the cathode performance with a goal of making sodium fuel cells with low cost, high energy, and long cycle life. Besides understanding the fundamental electrochemistry, I also develop novel material synthesis for scalable production of electrode materials and roll-to-roll manufacturing.

What would you like to do in your career?

I would like to expand my skills in doing scientific research where I can keep learning and growing. I enjoy the collaboration with scientists in multidisciplinary fields to solve problems. I would like to take on more responsibility in mentoring students besides developing ideas and completing my own research.

Why did you choose a career in science?

Growing up in a family of scientists, I was inspired all the time from my parents' conversations and birthday gifts (a hydrogen fuel cell car kit and a radio electronic DIY kit). I also had awesome mentors when I started doing research. Moreover, overcoming challenges to solve scientific puzzles is so fulfilling.

Syed Islam

Postdoc, Chemical Sciences Division
Ph.D., Chemical Engineering, University of Kentucky
Hometown: Comilla, Bangladesh

What are you working on at ORNL?

The focus of my research is the development of novel membrane technologies for the recovery and recycling of rare earth elements from electronic wastes including cellphones and hybrid/electric cars. It will meet the growing demand and address the supply risk of REEs for clean energy technologies.

What would you like to do in your career?

I would like to build a research program to develop next-generation, advanced, novel materials and processes for energy-efficient and highly selective separations and purifications in energy and environmental applications. The research will address global energy security challenges with environmentally friendly solutions.

Why did you choose a career in science?

I had an uncanny knack for doing mathematics from my elementary school. Growing up in a village, aspiring to live a prosperous life, and knowing science as creating something new led me to pursue science. With time I felt that I really loved to reflect on and find immense pleasure in doing science.

The church that's not supposed to be there

by Jim Pearce
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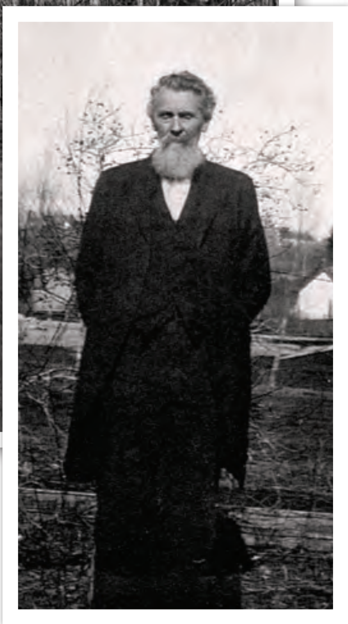
National laboratories have their share of odd structures. Often, these are architecturally impressive, state-of-the-art research facilities or relics of bygone R&D projects waiting to be dismantled.

But among ORNL's quirky structures is one that has little to do with science. In fact, it has survived for over 75 years in spite of science.

Stand across the street from ORNL's Physics building, and you will see an imposing granite monument bearing an unusual inscription: "Erected in Memory of New Bethel Baptist Church, Open 1851 Closed 1942 ... Church Building Stood 47 Feet in Front of this Stone."

If you then turn around, you can see what makes it so unusual. About 47 feet in front of you is a little white church that's not supposed to be there anymore.

Monument erected 47 feet from the church. Image credit, Carlos Jones, ORNL



New Bethel Baptist Church minister, the Rev. James Thomas Miller. Image courtesy Wanda Grubb Albers

The New Bethel Baptist Church was founded in 1851 in the small farming community of Scarborough. The community itself was established in the 1790s and was named after three brothers—Jonathan, David and James Scarborough—who were early settlers from Virginia. The area had previously been called Pellissippi by the Cherokee, and the church building that stands on the site today was built in 1924.

Unfortunately, the community didn't have a lot of time with its new building. In 1942, after the United States entered World War II, the federal government purchased 59,000 acres in the area for the construction of Manhattan Project facilities, forcing residents of Scarborough and several other small communities to relocate.

Assuming that the building would be torn down, church leaders voted to erect the granite memorial at the front of the hillside cemetery as their last official action. Yet somehow the church dodged the wrecking ball.

In the early years of the Manhattan Project, the building served as a planning office for construction of the Graphite Reactor—the world's first continually operating nuclear reactor. The reactor would eventually play a key role in scientific advancements ranging from the development of nuclear power and the field of neutron science to the production of medical radioisotopes for treating cancer.

In 1949, former church members were allowed to hold a final service and officially close the building as a house of worship.

Over the years, the church building was used for storage, temporary meeting space and even scientific experiments. When the church was added to the National Register of Historic Places in 1992, it reopened as an interpretive center and museum highlighting the Scarborough community. It underwent extensive repairs and restoration in 2004.

Today, the little white church is a regular stop on DOE's public bus tour of Oak Ridge facilities. More importantly, it's a reminder of the history and culture of the region and of the sacrifices made by ordinary citizens to support their country in a time of need.

New Bethel Baptist Church in 2015.
Image credit: Jim Richmond, ORNL

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OAK RIDGE NATIONAL LABORATORY REVIEW
PO Box 2008, Oak Ridge, Tennessee 37831-6266

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

ISSN 0048-1262