OAK RIDGE NATIONAL LABORATORY

Review

User facilities:

8 • World-class resources for the research community

OAK RIDGE National Laboratory

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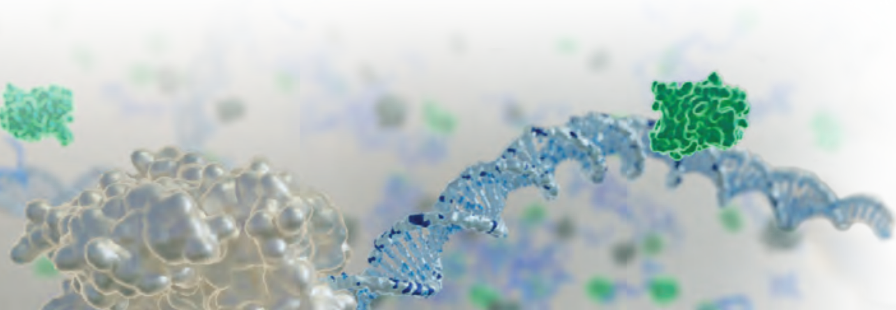
On the Cover

Vanderbilt University researcher Sami Halimi earned a Ph.D. based on experiments he conducted at ORNL's Center for Nanophase Materials Sciences. Image credit: Vanderbilt University School of Engineering



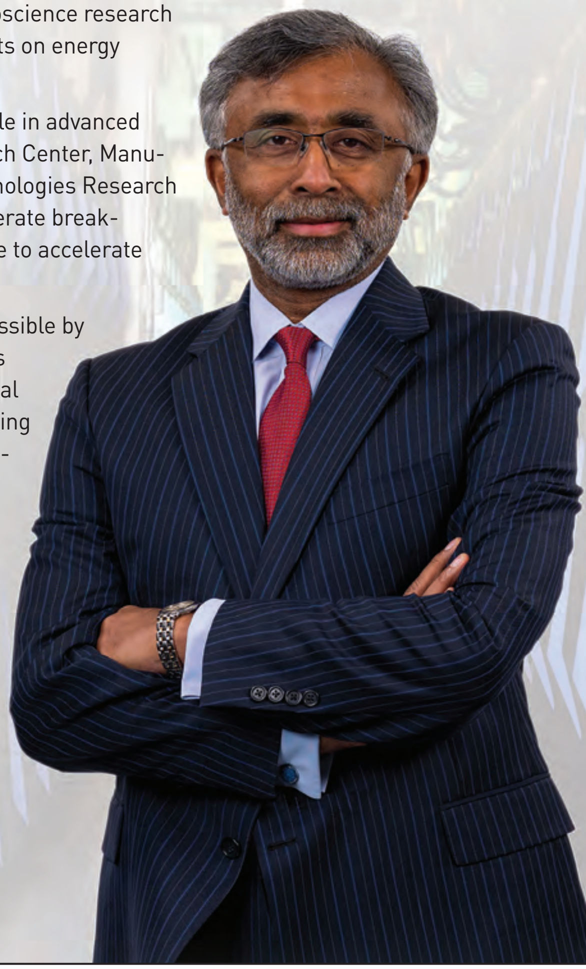
ORNL user facilities advance science and technology

One of the most important roles fulfilled by the Department of Energy's national laboratories is the construction and operation of unique and world-leading experimental facilities for use not just by national lab scientists but by the larger research community.

Oak Ridge National Laboratory has eight such facilities. They support diverse research priorities ranging from fundamental discoveries about the origins of the universe to practical advances in clean energy technology. These extraordinary facilities serve researchers from across the country and around the world, from academia, industry and other government labs, while helping ORNL scientists develop world-leading expertise in their fields.

The size and complexity of these facilities are largely beyond the means of even major research universities. This is especially true of facilities supported by DOE's Office of Science, including our Spallation Neutron Source, High Flux Isotope Reactor, Oak Ridge Leadership Facility, and Center for Nanophase Materials Sciences (see "Getting down to basic: Going big to study the very small," page 14, and "OLCF: Serving Up Bleeding-Edge Compute Power and Expertise to the World's Scientists," page 18).

SNS (the world's most powerful pulsed neutron source) and HFIR (the most powerful reactor-based source of neutrons in the United States) provide unique capabilities to the neutron science community. The OLCF, home to the world's most powerful supercomputer, Frontier, provides unprecedented opportunity to researchers in artificial intelligence and scientific supercomputing. And CNMS provides state-of-the-art equipment to support the nanoscience research that yields breakthroughs such as new materials that can have transformative impacts on energy and technology.



ORNL researchers in the applied sciences are pushing the envelope of what is possible in advanced manufacturing and clean energy technologies at our National Transportation Research Center, Manufacturing Demonstration Facility, Carbon Fiber Technology Facility and Building Technologies Research and Integration Center, and extensive partnerships with academia and industry accelerate breakthroughs to commercial applications (see "National user facilities use applied science to accelerate industry growth," page 22).

This issue of the *ORNL Review* will explain not only the remarkable research made possible by our user facilities but introduce you to some of our talented scientists and technicians and the visiting researchers who make the most of them (see "User facilities: Essential support for the country's researchers," page 8). Our experts are a boon to users working on site; they are an irreplaceable support for those who have had to access our instruments remotely during the travel restrictions of the COVID-19 pandemic.

Also in this edition of the *ORNL Review*, we look back at the ORNL career of Doris Scott, a Black nurse who was appointed in 1952 by President Truman to the Industrial Health Section of the President's Committee for Health (see "Nurse Doris Scott bridged lab's early race–health disparity," page 52).

We talk with ORNL Director of Technology Transfer Mike Paulus about the Lab's top 10 technology transfer successes (see "Mothers (and fathers) of invention: Getting ORNL tech into the world," page 38).

As always, we talk with postdocs and grad students about their work at ORNL and their plans for the future (see "Why Science?" page 50)

And we feature technical articles by ORNL staff members in Research Insights (see page 54). In this issue we discuss quantum science research at the Lab.

I hope you enjoy this issue of *ORNL Review*.

Thomas Zacharia

Thomas Zacharia
Laboratory Director

Frontier is world's fastest supercomputer

ORNL's newly installed Frontier supercomputer earned the top ranking as the world's fastest on the 59th TOP500 list released May 30. With 1.1 exaflops of performance, the system is the first to achieve exascale, a threshold of a quintillion calculations per second.

The Frontier system leverages ORNL's extensive expertise in accelerated computing and will enable scientists to develop critically needed technologies for the country's energy, economic and national security sectors, helping researchers address problems of national importance that were impossible to solve just five years ago.

"Frontier is ushering in a new era of exascale computing to solve the world's biggest scientific challenges," ORNL Director Thomas Zacharia said. "This milestone offers just a preview of Frontier's unmatched capability as a tool for scientific discovery. It is the result of more than a decade of collaboration among the national laboratories, academia and private industry, including DOE's Exascale Computing Project, which is deploying the applications, software technologies, hardware and integration necessary to ensure impact at the exascale."

Rankings were announced at the International Supercomputing Conference 2022 in Hamburg, Germany. Frontier's speeds surpassed those of any other supercomputer in the world, including ORNL's Summit, which at No. 4 on the TOP500 list continues as an impressive workhorse for open science.

Frontier, an HPE Cray EX supercomputer with AMD processors, also claimed the No. 1 spot on the Green500 list, which rates energy use and efficiency, with 62.68 gigaflops performance per watt. With 6.88 exaflops, Frontier also took the top spot in a newer category for mixed-precision computing, HPL-AI, that rates performance in formats commonly used for artificial intelligence.

ORNL's Frontier supercomputer. Image credit: Carlos Jones

Next steps for Frontier include continued testing and validation of the system, which remains on track for final acceptance and early science access later in 2022 and for full science at the beginning of 2023. — *Katie Bethea*

Materials tested in space for effects of radiation

To study how space radiation affects materials for spacecraft and satellites, ORNL scientists sent samples to the International Space Station. The results will inform the design of radiation-resistant magnetic and electronic systems.

Samples of four unique materials hitched a ride to space as part of an effort by ORNL scientists to evaluate how each fares under space conditions. Image credit: Zac Ward, ORNL

"Our aim is to explore the impact of harsh orbital environments on new classes of quantum materials," said ORNL's Zac Ward.

Four materials had the right stuff for the study. Gold will reveal how fast energetic ions etch a surface. An oxide crystal with many different randomly distributed atoms will show whether inherent disorder can protect a material's functional properties. An insulator with topologically protected conducting surface states will test the robustness of this protection from cosmic damage, and an antiferromagnet will indicate how electron spin alignment is influenced in space.

Launched in August 2021, the materials will be monitored in situ and retrieved in fall 2022 for postmortem characterization at ORNL. — *Dawn Levy*

Perovskite study points to better solar batteries

A study by ORNL researchers takes a fresh look at what could become the first step toward a new generation of solar batteries.

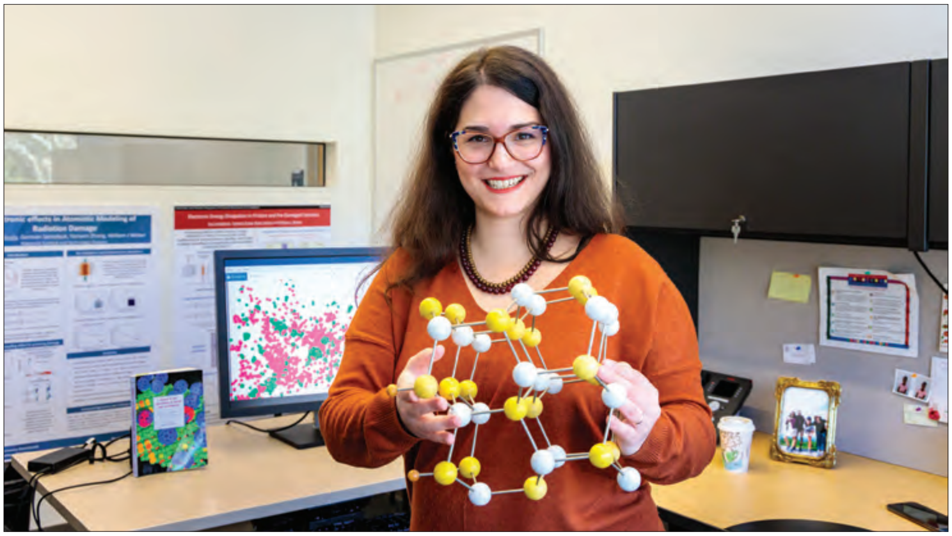
The study examines the structure of metal halide perovskites, a family of crystalline metals that are promising for their ability to turn light into electric energy, known as photovoltaic conversion. The study relied on the comprehensive expertise and state-of-the-art equipment of ORNL's Center for Nanophase Materials Sciences, or CNMS, to probe how that structure interacts with ions in motion, electric polarization and other phenomena to generate that energy. Results could point to techniques for designing more efficient, longer-lasting solar-cell batteries and other photovoltaic devices.

"These materials have mostly been studied under static conditions," said ORNL's Yongtao Liu, lead author of the study with ORNL's Olga Ovchinnikova. "We studied the materials in real time so we could understand such variables as how the ions are moving. You can't get a complete picture otherwise. Our findings suggest these ion migration patterns are key to efficiency in converting solar energy to power and the stability of the solar cells."

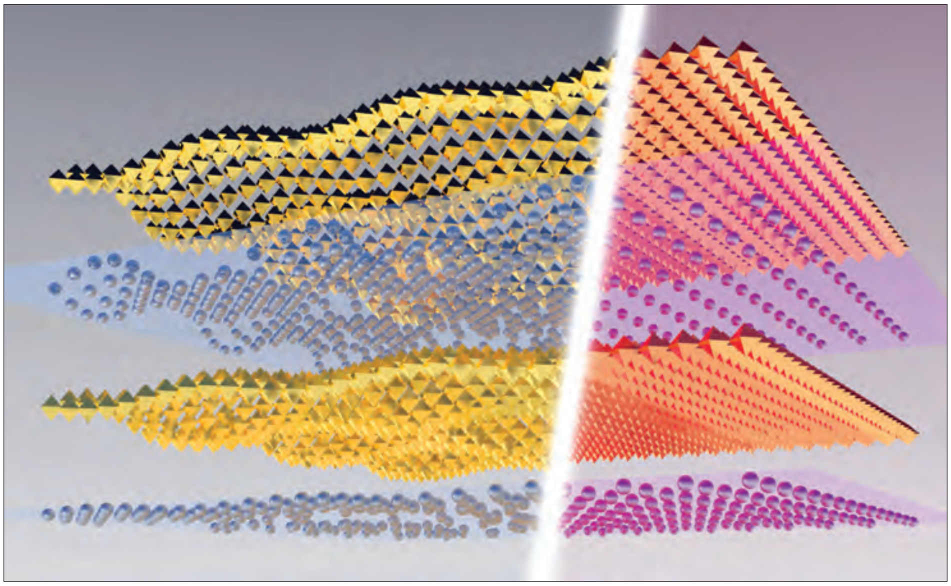
Metal halide perovskites became a focus of solar-cell research in recent years when studies revealed the materials' potential to offer untapped reservoirs of energy generated from light. The continuing search for clean, reliable power sources makes them a natural candidate for research.

"There's a huge interest in these materials because standard multicrystalline silicon-based solar cells have reached a peak conversion efficiency of about 23 percent over the past 40 years," said Ovchinnikova, who oversaw experiments while a staff member at the CNMS. "These metal halide perovskites have already surpassed that efficiency rate in the past decade alone." — *Scott Jones*

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



ORNL's Eva Zarkadoula investigates piezoelectric materials for use in sensors that can withstand irradiation, which causes cascading collisions that displace atoms and produces defects. Image credit: Carlos Jones, ORNL



This image illustrates lattice distortion, strain and ion distribution in metal halide perovskites, which can be induced by external stimuli such as light and heat. Image credit: Stephen Jesse, ORNL

Piezoelectric materials bombarded with neutrons

To advance sensor technologies, ORNL researchers studied piezoelectric materials, which convert mechanical stress into electrical energy, to see how they could handle bombardment with energetic neutrons. This irradiation disturbs the position and behavior of atoms, which can affect the conversion of mechanical stresses into electricity.

Sensors made of piezoelectric materials could help guide the design of prototype nuclear reactors and monitor the health of aging reactors — if the materials can withstand extreme conditions.

The researchers investigated aluminum nitride doped with scandium. Compared to undoped material, doped material had a heightened piezoelectric response and improved resilience to irradiation damage.

"With theory and experiment, we improved our understanding of how damage is induced in sensors inside a nuclear reactor and how irradiation affects the piezoelectric properties," said ORNL's Eva Zarkadoula, who led the study.

Zarkadoula hopes the new knowledge advances tools to improve nuclear reactors, America's largest source of carbon-free energy. — *Dawn Levy*

Govindarajan Muralidharan

ORNL's Muralidharan joins national academy

Govindarajan Muralidharan, a scientist and inventor at ORNL, has been elected a fellow of the National Academy of Inventors.

The NAI was established to recognize inventors with U.S. patents and to promote academic technology and innovation that globally benefits society. NAI fellows have achieved the highest professional distinction accorded solely to academic inventors.

Muralidharan was recognized for "a highly prolific spirit of innovation in creating or facilitating outstanding inventions that have made a tangible impact on the quality of life, economic development and welfare of society."

Muralidharan is a distinguished staff member in the Metals and Composites Processing Group for ORNL's Materials Science and Technology Division, where his research focuses on structural materials, functional materials and sensors.

He has made significant contributions to the research, development and commercialization of high-temperature alloys for use in harsh environments prevalent in many industrial processes, nuclear systems and combustion engines. — *Ashley Huff*

For more information: https://go.usa.gov/xzHC4

Lignin research points to cheaper biofuels

A team of researchers working within the Center for Bioenergy Innovation at ORNL has discovered a pathway to encourage a type of lignin formation in plants that could make the processing of crops grown for products such as sustainable jet fuels easier and less costly.

The researchers focused on C-lignin, a polymer in the seed coats of certain exotic plants. Lignin, the polymer that gives plants their rigidity, is a good source of the building blocks and aromatic chemical compounds needed to produce clean bio-based fuels. But lignin is also difficult to process, particularly the more common G-lignin and S-lignin found in most plants.

C-lignin has a chemical structure that is more linear than the other lignins, making it easier to deconstruct. The scientists working as part of CBI have now identified the genetic mechanism at play in the formation of this preferred C-lignin, as detailed in *Science Advances*. The scientists hope to engineer bioenergy crops to form C-lignin while constraining the growth of G-lignin and S-lignin, which could lead to more affordable, higher-yield bioprocessing.

G-lignin and S-lignin form polymer structures much like a fishing net with branches and kinks in it, while C-lignin is more of a string, explained Jerry Tuskan, CBI's chief executive officer. "You can imagine that it would be harder to pull apart a fishing net than a string that just unravels."

Moving forward, Tuskan said the researchers want to engineer this polymer into their primary feedstocks of poplar trees and switchgrass as a means of making their cell walls easier to break down for conversion into sustainable aviation fuels. — *Kim Askey*

ORNL's Elliott honored with Smithsonian statue

ORNL scientist Amy Elliott is one of 120 women who were featured in a novel exhibit, "IfThenSheCan," at the Smithsonian to commemorate Women's History Month.

A life-sized 3D-printed statue of Elliott, a manufacturing scientist, was on display in the Smithsonian Castle in Washington, D.C., through March 27. The statues recognized women who have excelled in STEM fields — science, technology, engineering and mathematics — and was the largest collection of statues of women ever assembled.

Elliott, who leads ORNL's Robotics and Intelligent Systems Group, specializes in the inkjet-based 3D printing of metals and ceramics, a technology designed to enhance and transform advanced manufacturing in the automotive, aerospace and power generation sectors. Her inventions have been licensed by industry and have won prestigious awards including two R&D 100 Awards. She also holds several patents and licenses, including a

A greenhouse research facility at ORNL used in the development of advanced bioenergy crops.
Image credit: Carlos Jones, ORNL

ORNL's Amy Elliott was among women in STEM featured with a life-sized statue in the Smithsonian exhibit, "IfThenSheCan," to commemorate Women's History Month. Image credit: Amy Elliott, ORNL

method for 3D metal printing and additive manufacturing of aluminum boron carbide metal composites.

"As a 3D-printing researcher, it was so cool to get 3D-scanned for the statue and printed while expecting my first child," Elliott said. "I love being a STEM mom and feel so honored to be part of history and the IfThenSheCan exhibit." — *Sara Shoemaker*

For more information: https://go.usa.gov/xzH2M

New analyzer a step toward quantum internet

Researchers at ORNL, SRI International, Freedom Photonics and Purdue University have made strides toward a fully quantum internet by designing and demonstrating the first-ever Bell state analyzer for frequency bin coding.

Before information can be sent over a quantum network, it must first be encoded into a quantum state. This information is contained in qubits, or the quantum version of classical computing "bits" used to store information, that become entangled, meaning they reside in a state in which they cannot be described independently of one another.

Entanglement between two qubits is considered maximized when the qubits are said to be in "Bell states."

Measuring qubits' Bell states is critical to many of the protocols necessary to perform quantum communication and distribute entanglement across a quantum network. And while these measurements have been done for many years, the team's method represents the first Bell state analyzer developed specifically for frequency bin coding, a quantum communications method that harnesses single photons residing in two different frequencies simultaneously.

"Measuring these Bell states is fundamental to quantum communications," said ORNL's Joseph Lukens. "To achieve things such as teleportation and entanglement swapping, you need a Bell state analyzer."

Teleportation is the act of sending information from one party to another across a significant physical distance, and entanglement swapping refers to the ability to entangle previously unentangled qubit pairs.

The analyzer was designed with simulations and has demonstrated 98% fidelity; the remaining 2% error rate is the result of unavoidable noise from the random preparation of the test photons and not the analyzer itself, Lukens said. This incredible accuracy enables the fundamental communication protocols necessary for frequency bins, a previous focus of Lukens' research. — *Scott Jones*

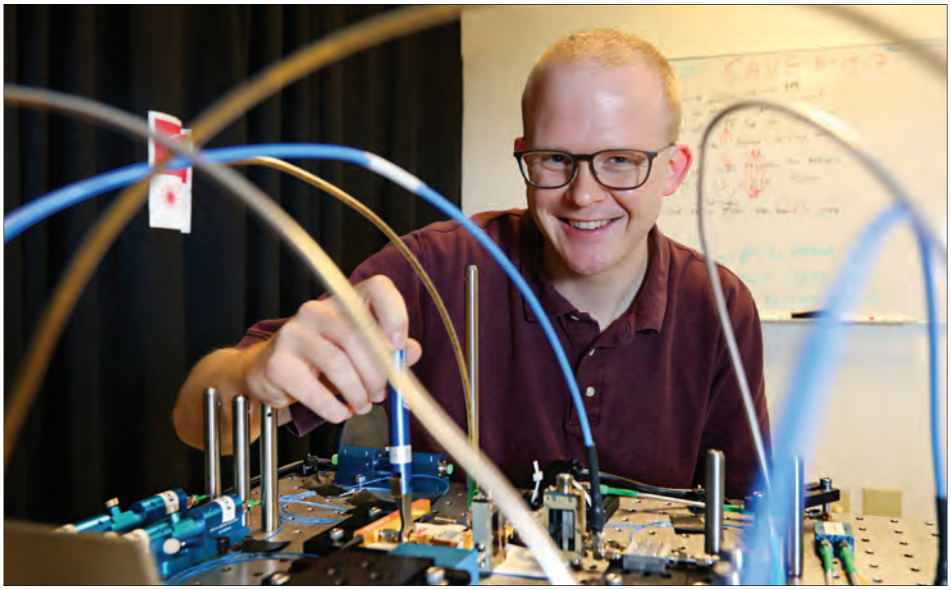
For more information: https://go.usa.gov/xzHTM

ORNL-led study could lead to point-and-click design

An ORNL-led study could help make materials design as customizable as point-and-click.

The study, published in *npj Computational Materials*, used an invertible neural network, a type of artificial intelligence that mimics the human brain, to select the most suitable materials for desired properties, such as flexibility or heat resistance, with high chemical accuracy. The team's findings offer a potential blueprint for customizing scientific design and speeding up the journey from drawing board to production line.

"These results are a really nice first step to expanding capabilities for materials design," said Victor Fung, until recently a Eugene Wigner fellow at ORNL's Center for Nanophase Materials Sciences and lead author of the study. "Instead of taking a material and predicting its given proper-



ORNL's Joseph Lukens runs experiments in an optics lab. Image credit: Jason Richards, ORNL ties, we wanted to choose the ideal properties for our purpose and work backward to design for those properties quickly and efficiently with a high degree of confidence. That's known as inverse design."

Neural networks rely on millions of digital neurons and synapses similar to those in the brain. The neurons can operate independently and don't necessarily perform calculations in traditional ways. The neurons of an invertible neural network operate in one-to-one pairs like tag teams, a process known as bijective function approximation.

The inverse design approach used in the study leverages advances in the invertible neural architecture to enable forward mapping, which adds up input to produce a result, and backward mapping, which starts with a result and works back to deduce the initial input. — *Matt Lakin*

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

ORNL tech licensed to make batteries safer

Several electrolyte and thin-film coating technologies developed at ORNL have been licensed by BTRY, a battery technology company based in Virginia, to make batteries with increased energy density, at lower cost and with an improved safety profile in crashes.

The enabling technologies, called Safe Impact Resistant Electrolytes, or SAFIRE, are particularly suitable for application in the electric vehicle and aerospace industries.

"In a lithium-ion battery, a thin piece of plastic separates the two electrodes," said ORNL's Gabriel Veith. "If the battery is damaged and the plastic layer fails, the electrodes can come into contact and cause the battery's liquid electrolyte to catch fire."

ORNL's technology mixes an additive into the conventional electrolyte to create an impact-resistant electrolyte. It solidifies when hit, preventing the electrodes from touching if the battery is damaged. This new stability reduces the need for bulky protective shielding. — *Karen Dunlap*

Wullschleger honored for commitment to diversity

Stan Wullschleger, ORNL's associate laboratory director for biological and environmental systems science, is the recipient of the 2022 Commitment to Human Diversity in Ecology Award from the Ecological Society of America, or ESA.

The award honors Wullschleger for his long-standing contributions to increasing diversity in the future generation of ecologists through mentoring, teaching and outreach.

"In 30 years of experience, Dr. Wullschleger interacted with hundreds of scientists, technicians and students, providing leadership, strategic planning and professional development opportunities," the ESA stated. "We honor him for the initiatives to create an inclusive and diversified culture among scientists while bringing awareness to the discipline and ecological profession."

The ESA awards committee noted that Wullschleger's career is "marked by his commitment to providing opportunities, safe spaces and highlighting the contributions of different ethnic groups, gender identities and cultures."

In addition to leading ORNL's Biological and Environmental Systems Science Directorate, Wullschleger is an ORNL Corporate Fellow and oversees the lab's Climate Change Science Institute. He also directs the DOE's Next-Generation Ecosystem Experiments Arctic project, or NGEE Arctic, a long-term endeavor exploring the function of tundra ecosystems in a rapidly changing climate.

"I am deeply honored to receive this award from the Ecological Society of America," Wullschleger said. "Throughout my career, I have benefited from the insight and inspiration of my colleagues. Our teams must increasingly embrace diverse views, perspectives and life experiences as together we push the frontiers of scientific knowledge forward. It is essential that everyone be included, heard and valued as we interact to better understand, predict and develop strategies to address environmental change." — *Kim Askey*

Stan Wullschleger

Microscopy technique focused on lithium

ORNL researchers have demonstrated an electron microscopy technique for imaging lithium in energy storage materials such as lithium-ion batteries at the atomic scale.

The properties of energy storage materials stem directly from their atomic structures, which are only visible using electron microscopy. Today's advanced electron microscopes are able to image heavy elements at atomic resolution. One challenge is simultaneously observing light elements including lithium, sodium and potassium, which are essential for modern batteries.

Scientists at ORNL's Center for Nanophase Materials Sciences used "center-of-mass" scanning transmission electron microscopy, or CoM-STEM, to observe lithium along with heavier elements in battery materials at atomic resolution.

"Imaging light and heavy elements together is important for advancing energy storage materials, but many techniques require significant expertise or yield data that are difficult to interpret," said

ORNL's Michael Zachman. "CoM-STEM is a straightforward technique that will now be more accessible across the research community." — *Ashley Huff*

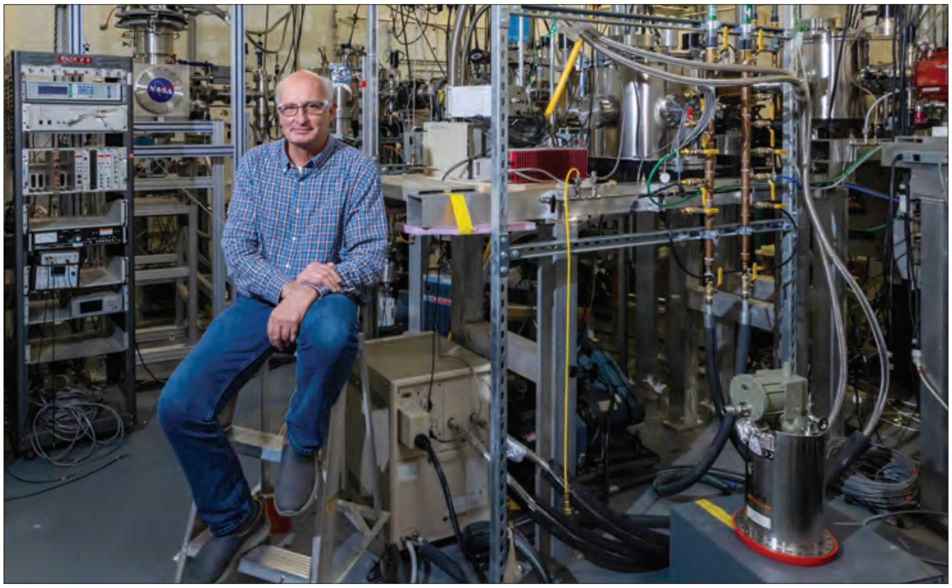
ORNL facility examines cosmic origins of X-rays

Scientists are using ORNL's Multicharged Ion Research Facility to simulate the cosmic origin of X-ray emissions resulting when highly charged ions collide with neutral atoms and molecules, such as helium and gaseous hydrogen.

"This facility gives us a new X-ray observational window to peer into otherwise invisible processes found in star-forming galaxies, galaxy clusters, supernova remnants and relativistic jets from black holes," said ORNL's Charles Havener.

Havener and collaborators developed techniques to collide beams of ions with neutral atoms or molecules present in space. They measure X-ray emissions from charge–exchange processes using an X-ray quantum calorimeter developed at the University of Wisconsin with NASA Goddard Space Flight Center. Its high resolution will enable improved understanding of astrophysical processes.

"In the future, we want to measure X-ray emissions from charge exchange with atomic hydrogen, the most abundant element in the universe, but the most challenging measurement in a lab," Havener said. — *Dawn Levy*



ORNL physicist Charles Havener uses the NASA end station at ORNL's Multicharged Ion Research Facility to simulate the origin of X-ray emissions from space. Image credit: Carlos Jones, ORNL

UT-Battelle Scholarship recipient James Rogers, second from right, and parents David, left, and Melanie Rogers are congratulated by ORNL Director Thomas Zacharia. Image credit: Carlos Jones, ORNL

High school senior wins UT-Battelle scholarship

Oak Ridge High School senior James Rogers has been named recipient of the 2022 UT-Battelle Scholarship to attend the University of Tennessee.

The competitive scholarship is awarded annually to a graduating senior who is planning to study science, mathematics or engineering at UT and who has a parent employed by UT-Battelle, ORNL's managing contractor. The scholarship is renewable for up to four years and is worth a total of $20,000.

Rogers is the son of David and Melanie Rogers of Oak Ridge. David is a research and development staff member in ORNL's National Center for Computational Sciences.

Rogers has expressed a passion for physics that led him to form and lead a Students of Undergraduate Physics club at ORHS. He plans to focus on plasma physics in college because of the field's application to fusion energy and the production of clean energy.

He completed the Austin Peay State University School for Computational Physics in 2021, which he says showed him the value of collaboration and building good working relationships.

"As an apprentice/employee and as a leader, I want to contribute to the maintenance of a collaborative environment in my workplace, but also to spread my appreciation of collaboration to others by always being humble, as humility and whimsy are key aspects of a productive work environment," Rogers wrote in his essay. — *Bill Cabage*

ORNL user facilities

Oak Ridge Leadership Computing Facility

Established in 1992, the OLCF is home to the newly installed Frontier, the world's most powerful supercomputer, and to Summit, which was until recently the nation's most powerful system. Summit can perform 200 million billion calculations every second. Frontier is nearly 10 times more powerful, able to perform more than a billion billion calculations each second.

Notable accomplishment: Modeled an aerosolized SARS-CoV-2 viral particle for the first time, placing it in a 1.05-billion-atom system, one of the largest biochemical systems ever simulated at the atomic level.

High Flux Isotope Reactor

Completed in 1965 and operating at 85 megawatts, HFIR's steady-state neutron beam is the strongest reactor-based neutron source in the United States. The thermal and cold neutrons produced by HFIR are used to study physics, chemistry, materials science, engineering and biology.

Notable accomplishment: Revealed at the molecular level how a key protein from the SARS-CoV-2 virus (the papain-like protease, or PLpro) links up with the human protein interferon-stimulated gene 15 to evade the body's immune response.

User facilities:

Essential support for the country's researchers

by Leo Williams
williamsjl2@ornl.gov

U.S. Forest Service researcher Nayomi Plaza had an important question: What happens to wood at the molecular level when it's exposed to humidity?

The answer will give us a better understanding of the movement of water in lumber, allowing us to choose better anti-decay treatments and improve the lumber for construction and other uses.

To find it, Plaza chose neutron scattering — a technique that's uniquely good at studying the behavior of water.

Since the Forest Products Laboratory does not have the equipment to perform needed neutron scattering tests, Plaza partnered with ORNL and its world-leading neutron facilities — the accelerator-based Spallation Neutron Source and the reactor-based High Flux Isotope Reactor — to address these research questions.

"My work supports the Forest Service mission of sustaining our nation's forests and grasslands by unlocking the potential of wood, our most abundant and renewable resource" Plaza said, "and ORNL is instrumental to my research."

Bringing in researchers

SNS and HFIR are just two of eight ORNL user facilities that help researchers from around the country and around the world

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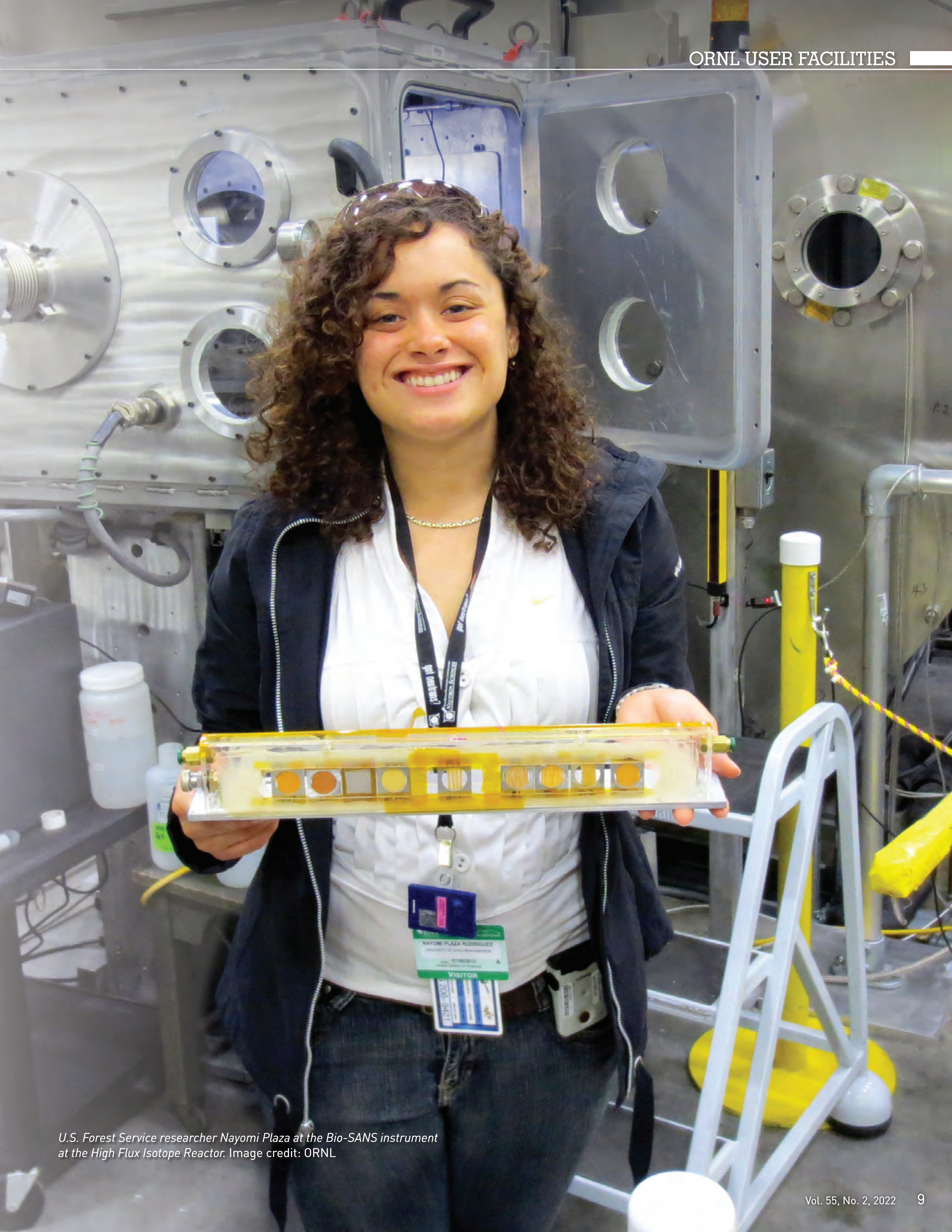

U.S. Forest Service researcher Nayomi Plaza at the Bio-SANS instrument at the High Flux Isotope Reactor. Image credit: ORNL

Spallation Neutron Source

Opened in 2006, the SNS produces neutrons with a linear accelerator–based system that delivers short (microsecond) proton pulses to a steel target filled with liquid mercury. Each proton that collides with a mercury atom knocks loose 20–30 neutrons through a process called spallation. Those neutrons are then directed toward state-of-the-art instruments that provide a variety of capabilities to researchers across a broad range of disciplines, such as physics, chemistry, biology and materials science.

Notable accomplishment: Observed evidence for magnetic Majorana fermions associated with materials exhibiting long-sought Kitaev quantum spin liquid behavior. Theory suggests that such particles might serve as the basis of "qubits" for use in quantum computers.

Center for Nanophase Materials Sciences

Established in 2005, CNMS gives users access to staff expertise and state-of-the-art equipment for a broad range of nanoscience research, including nanomaterials synthesis; nanofabrication; imaging, microscopy and characterization; and theory, modeling and simulation.

Notable accomplishment: Allowed researchers to open new frontiers in controllable molecules by using a scanning tunneling microscope to move a single molecule between two independent probes and observe it disappear from one point and instantaneously reappear at the other.

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by giving them access both to world-leading resources they couldn't possibly afford and to expert staff that ensure they take full advantage of those facilities.

ORNL user facilities advance research in a wide range of science and technology, from explorations of the nature of the universe and its origins to the development of advanced manufacturing technologies that keep the United States competitive.

SNS and HFIR are among the lab's premier user facilities. Along with the Oak Ridge Leadership Computing Facility — home to the world's most powerful supercomputer, Frontier — and the Center for Nanophase Materials Sciences, they are sponsored by DOE's Office of Science (see "Getting down to basic: Going big to study the very small," page 14, and "OLCF: Serving up bleeding-edge compute power and expertise to the world's scientists," page 18).

> *"A lot of the work that we're doing with Oak Ridge is to help push the envelope as far as capabilities go: the materials that can be printed, the speed at which things can be printed, controlling the depositions for quality and accuracy.*
>
> — Business development manager for Lincoln Electric Additive Solutions **D. Mark Douglass**

"The Department of Energy is the major funder of physical sciences in the United States," noted ORNL Laboratory Director Thomas Zacharia. "One of the main functions of the Office of Science is to enable scientific discoveries and technological advances by providing unique user facilities not only to ORNL scientists, but to collaborators from across the United States and even around the world."

Arizona State University molecular biophysicist Abhishek Singharoy uses ORNL's Summit supercomputer, ranked fourth fastest in the world, to study the behavior of proteins in living cells, focusing on mitochondria, a cell's components for producing energy, and on viruses and vaccines. His work offers insights into the aging process as well as the treatment of viral infections.

The molecular dynamics simulations that his team performs are extremely demanding, requiring a supercomputer of Summit's abilities.

"The kinds of simulations we do involve millions of variables," he said, "and each variable has basically six dimensions that need to be monitored. That brings us to 6 million to 60 million variables that need to be monitored every millisecond of the calculation."

Singharoy's research also benefits from Summit's strengths in machine learning and artificial intelligence, which streamline

See USER FACILITIES: ESSENTIAL SUPPORT, page 12

> "The OLCF staff have been amazing. Working with them has been a pleasure. Anytime we get stuck somewhere, the OLCF staff have been extremely helpful, working with us hand-in-hand toward solving these problems.
>
> — Arizona State University molecular biophysicist **Abhishek Singharoy**

Arizona State University molecular biophysicist Abhishek Singharoy uses ORNL's Summit supercomputer to study the behavior of proteins in living cells. Image credit: Arizona State University

Building Technologies Research and Integration Center

Established in 1993, BTRIC is the only DOE-designated national user facility devoted to building technologies research and development. The 60,000-square-foot campus includes the flagship MAXLAB, a multipurpose laboratory to advance the energy efficiency and durability of building envelopes, equipment and materials.

Notable accomplishment: Developed and demonstrated a new concrete mix that takes 15 percent less energy to manufacture than standard concrete, reduces by 40 percent the amount of concrete needed in precast insulated panels and doubles the production capacity of precast plants without capital investment.

Carbon Fiber Technology Facility

Established in 2013, the 42,000-square-foot CFTF focuses both on carbon fiber precursors — the materials that are turned into carbon fiber — and the ovens and other processing equipment needed to turn those precursors into usable carbon fiber.

Notable accomplishment: Collaborated with industry to produce enough specialty filter media to supply more than 1 million face masks and respirators each day to American health care facilities for the ongoing COVID-19 pandemic, including the development of a novel, in-line charging device to mass-produce precursor material for N95 masks.

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simulations on the fly, allowing Singharoy and his colleagues to tackle even more challenging problems.

"Summit allows us to think about problems that were previously unthinkable," he said.

Helping the economy with advanced tech

The lab also hosts user facilities dedicated to applied research. Sponsored by DOE's Office of Energy Efficiency and Renewable Energy, these include the Building Technologies Research and Integration Center, the Carbon Fiber Technology Facility, the Manufacturing Demonstration Facility and the National Transportation Research Center.

Cleveland, Ohio-based Lincoln Electric is one user taking advantage of ORNL's expertise in applied research. The company collaborates with the MDF to develop and improve metal 3D printing for heavy industries such as power plants and oil and gas refineries. Specifically they're focused on large machines that produce components using additive manufacturing with melted wire.

> *"What makes ORNL and these user facilities unique is not just their capability; it's the people — the scientists and technicians. When collaborators engage the user facilities, they are interacting not only with the equipment but also with extraordinary scientists and technicians who are part of our staff.*
>
> — ORNL Laboratory Director **Thomas Zacharia**

"A lot of the work that we're doing with Oak Ridge is to help push the envelope as far as capabilities go: the materials that can be printed, the speed at which things can be printed, controlling the depositions for quality and accuracy," said D. Mark Douglass, business development manager for Lincoln Electric Additive Solutions.

That relationship also gives the company access to the lab's neutron scattering facilities, which allow them to ensure the quality of the printed parts by checking for stresses and defects.

"Much of our effort is in characterizing the material," Douglass said. "What's the residual stress like? What are the mechanical properties like? What kind of discontinuities — some people call them defects — would you expect, and how do you control or minimize those?"

Lincoln also relies on ORNL for other testing. For instance, it's working with an iron–nickel alloy called Invar, which resists expansion and contraction when it is heated and cooled — a quality known as a low coefficient of thermal expansion.

"We would deposit various samples of different chemistries, and then the lab would test those chemistries for the critical variable, namely the coefficient of thermal expansion."

As always, it's about the people

Zacharia stressed that the value of ORNL's user facilities goes well beyond their technical capabilities to the expertise and commitment of their staff. These collaborations ensure that researchers make the most of these unique facilities, maximizing their impact on science and technology.

"What makes ORNL and these user facilities unique is not just their capability; it's the people — the scientists and technicians. When collaborators engage the user facilities, they are interacting not only with the equipment but also with extraordinary scientists and technicians who are part of our staff."

These collaborations were especially valuable during the pandemic, he noted.

"In the last two years, much of the work has been done by our staff, because the users simply they could not be here themselves." Zacharia said.

Plaza, Singharoy and Douglass agree.

Plaza's neutron research into wood and humidity used custom-made humidity chambers that allowed her to observe at the nanoscale how water moves in wood, how the wood swells when exposed to water, and how the process is affected by the treatments used to prevent decay.

"The people at ORNL have been absolutely wonderful," she said. "They've been super helpful as we've worked together coming up with new humidity cell environments so that I can do my experiments with humidity control."

Singharoy also praised his ORNL collaborators.

"The OLCF staff have been amazing," he said. "Working with them has been a pleasure. Anytime we get stuck somewhere, the OLCF staff have been extremely helpful, working with us hand-in-hand toward solving these problems."

Jason Flamm, engineering and operations manager for Lincoln Electric Additive Solutions, praised MDF staff both for their strength as collaborators and their help in getting the company access to the lab's neutron scattering facilities.

"MDF is a world-renowned expert in the area of additive manufacturing, especially large-scale additive manufacturing," he said. "They've got many knowledgeable people with lots of experience and breadth of experience."

Douglass also said he appreciated the perspective of ORNL's researchers, who are able to take a longer-term approach to technology development.

"Oak Ridge has the ability to look out into the future and have a longer horizon with some of the applications they're looking at. We wouldn't necessarily be giving them the same attention because of the demands of business."

Manufacturing Demonstration Facility

Established in 2012, the MDF focuses on early-stage research and development to improve the energy and material efficiency, productivity and competitiveness of American manufacturers. Research focuses on manufacturing analysis and simulation, composites and polymer systems, metal powder systems, metrology and characterization, machine tooling, large-scale metal systems and robotics and automation.

Notable accomplishment: Created the first 3D-printed thermal protection shield for use in a space mission, launched in August 2021 to the International Space Station.

National Transportation Research Center

Established in 2000, NTRC is DOE's only dedicated user facility focused on transportation. Researchers identify new materials for next-generation systems; provide decision-making tools and intelligent technologies for the secure, efficient movement of passengers and freight; and create economic opportunity for the nation by improving the energy efficiency of light-, medium- and heavy-duty vehicles.

Notable accomplishment: Developed a hands-free wireless charging technology that delivers high levels of power in a compact system to support fast, convenient, hands-free charging of electric vehicles.

Getting down to basic:

Going big to study the very small

by Paul Boisvert
boisvertpl@ornl.gov

A reality in science today is that in order to study the smallest, most fundamental elements of nature, scientists need access to some of the world's largest and most powerful research centers — with facilities often costing billions of dollars.

The instruments and supporting technologies at these facilities are necessary to explore the atomic, subatomic, and quantum structures and processes that form the most basic physical properties of materials and chemical processes.

> *"Observing and understanding the fundamental nature of materials typically doesn't lead immediately to developing and using the materials in everyday applications. But in the future, scientists can take today's discoveries and build on them to develop new and practical applied technologies.*
>
> — Georgia Tech associate professor **Martin Mourigal**

Unlike research in many other areas, the discoveries enabled by these explorations often don't have immediate practical application. Rather, they give us insight into how the universe is put together.

"Observing and understanding the fundamental nature of materials typically doesn't lead immediately to developing and using the materials in everyday applications," said Martin Mourigal, associate professor at Georgia Tech. "But in the future, scientists can take today's discoveries and build on them to develop new and practical applied technologies."

Mourigal and his students are frequent users of ORNL's neutron science facilities, where they study the basic properties of both natural and manmade materials.

"Basic science, or fundamental science, primarily involves the pursuit of knowledge purely for knowledge's sake," he said. "It differs from applied science in that it can take years or decades to employ basic science discoveries for practical purposes."

At ORNL, the Spallation Neutron Source, High Flux Isotope Reactor and Center for Nanophase Materials Sciences are user facilities devoted primarily to basic research. These facilities serve the global scientific community's pursuit of fundamental science questions and challenges. All three are supported by the DOE Office of Science, the single largest supporter of basic research in the physical sciences in the United States.

SNS is based on a nearly 1,000-foot-long linear accelerator and is one of the most powerful neutron sources in the world. The accelerator delivers a 1.4-megawatt pulsed stream of protons at nearly 90 percent of the speed of light to enable the world-class capabilities of its 19 neutron instruments.

SNS provides researchers with neutron beams that permit high resolution and a broad range of energies to use in experiments. The pulsed neutrons SNS produces are called "thermal" neutrons because their energy matches that of the jiggling motion of atoms at room temperature. Thermal neutrons have wavelengths of a few tenths of a nanometer, ideal for experiments such as determining the positions of atoms in solids and chemical reactions. Such studies have led to better understanding of phenomena such as magnetic order, superconductivity, and thermoelectricity in a variety of materials.

Complementing the SNS is the High Flux Isotope Reactor, an 85-megawatt nuclear reactor in which nuclear fission produces a steady stream of neutrons as a byproduct.

HFIR produces both thermal and "cold" neutrons, which are labeled as cold because they are passed through a cryogenically cooled moderator containing liquid hydrogen. This slows them down to produce less-energetic, longer-wavelength neutrons better suited for examining materials with lower-energy motions of atoms and magnetic interactions as well as larger structures — for example, the magnetic fluctuations in quantum materials or the spacing between groups of atoms in a protein.

In a typical year, the SNS and HFIR combine to host about 1,300 users from academia, industry and government who travel across the nation and from around the world to access these unique user facilities. The scientists have used the neutrons at SNS and HFIR

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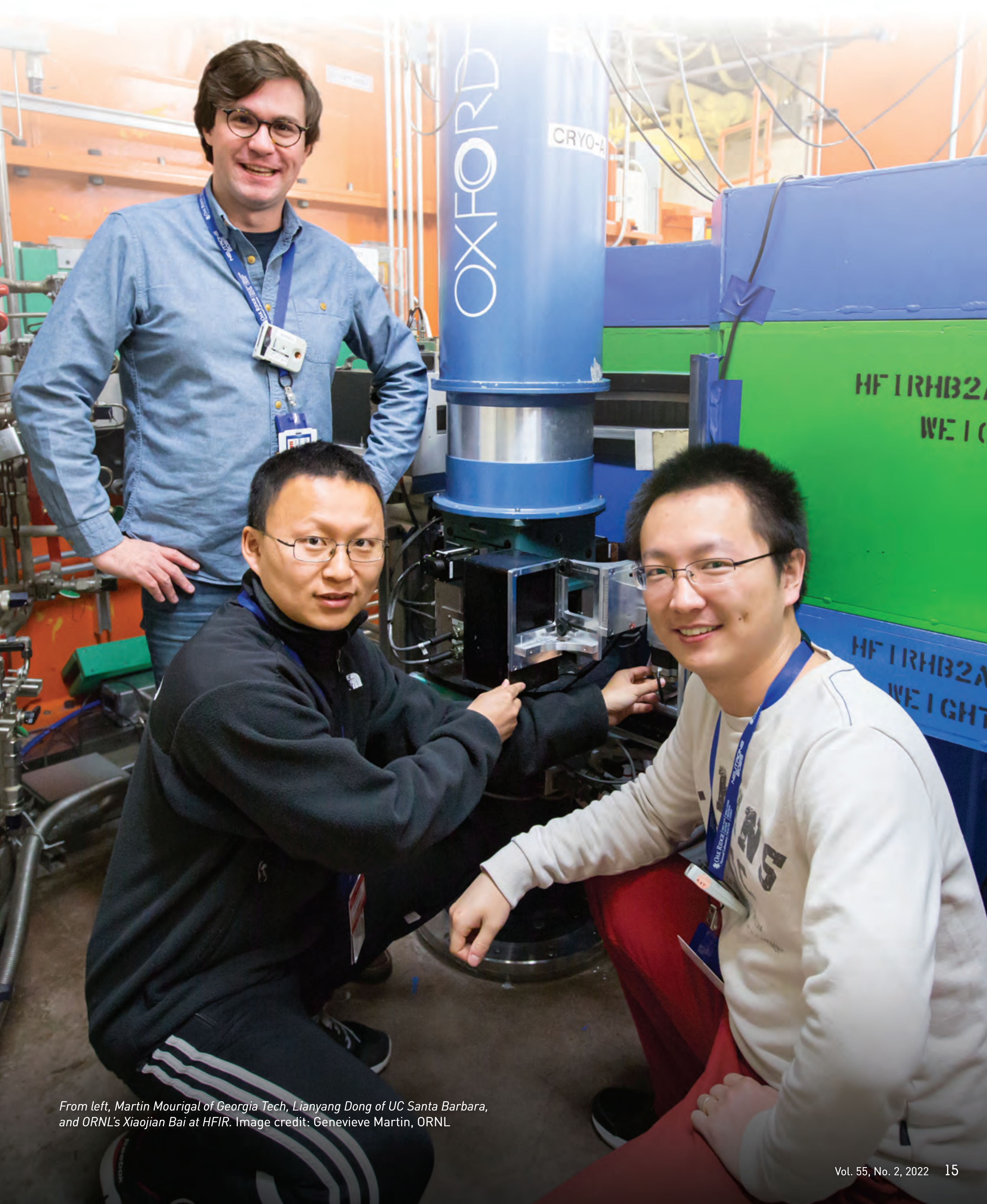


From left, Martin Mourigal of Georgia Tech, Lianyang Dong of UC Santa Barbara, and ORNL's Xiaojian Bai at HFIR. Image credit: Genevieve Martin, ORNL

GETTING DOWN TO BASIC, page 14

to achieve breakthrough discoveries in materials science, such as in materials used for energy storage, medicines and vaccines, polymers and many other applications.

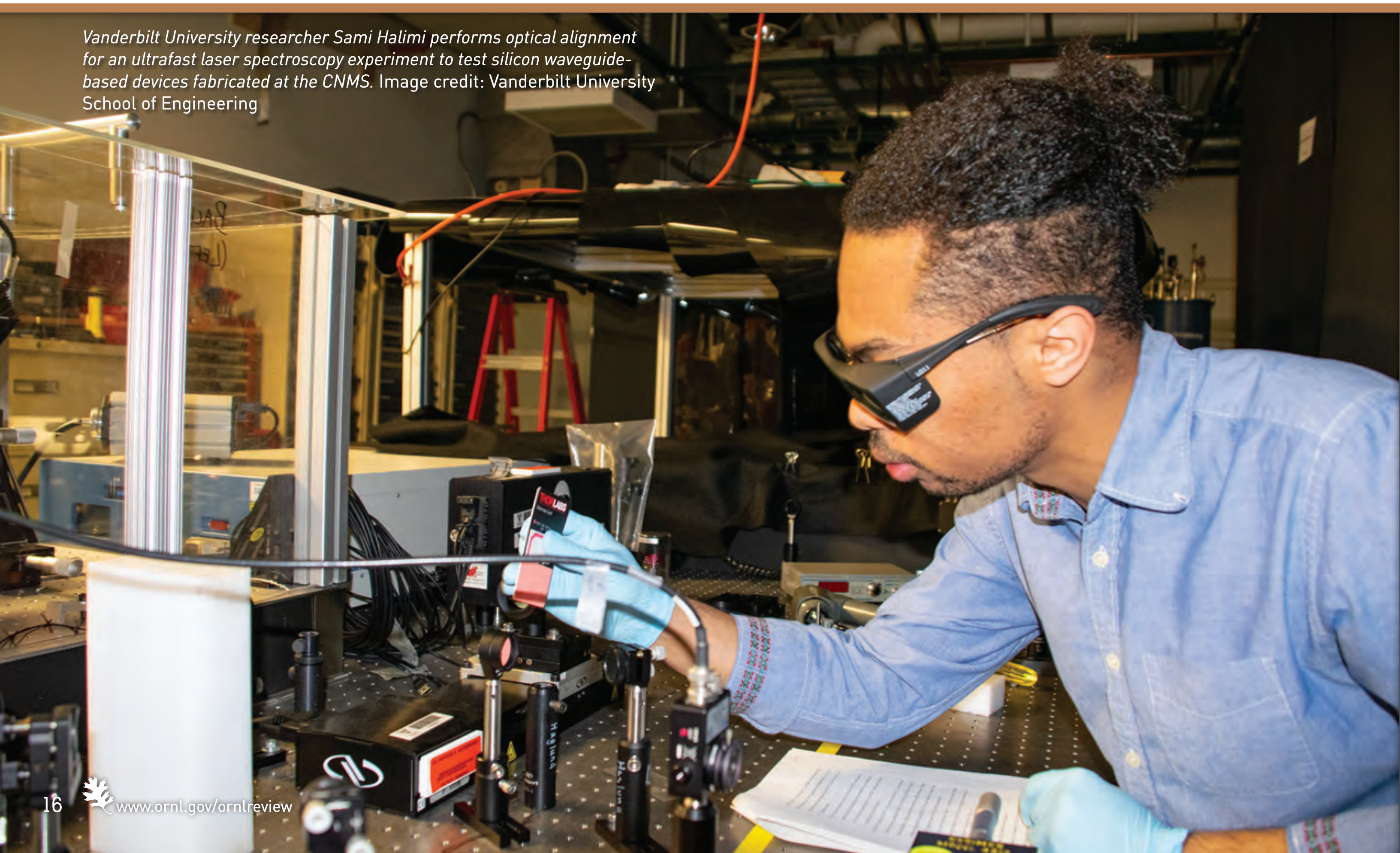
Neutrons are especially useful for observing lighter elements, such as hydrogen atoms, inside materials and biological samples. This makes neutrons ideal for many experiments, such as tracking the location of lighter atoms in lithium compounds inside batteries — typically without compromising or harming the samples.

"Our group's research at the SNS and HFIR is considered basic research because we investigate the behavior of electrons and atoms in materials," Mourigal said. "That's the grand challenge of basic science — predicting the behavior of matter, energy, and information from the laws of quantum mechanics that guide interactions between microscopic constituents. Without the unique, world-class capabilities of the SNS and HFIR, we could not do that research. We would simply not be able to study the materials and make discoveries as we've done over the years."

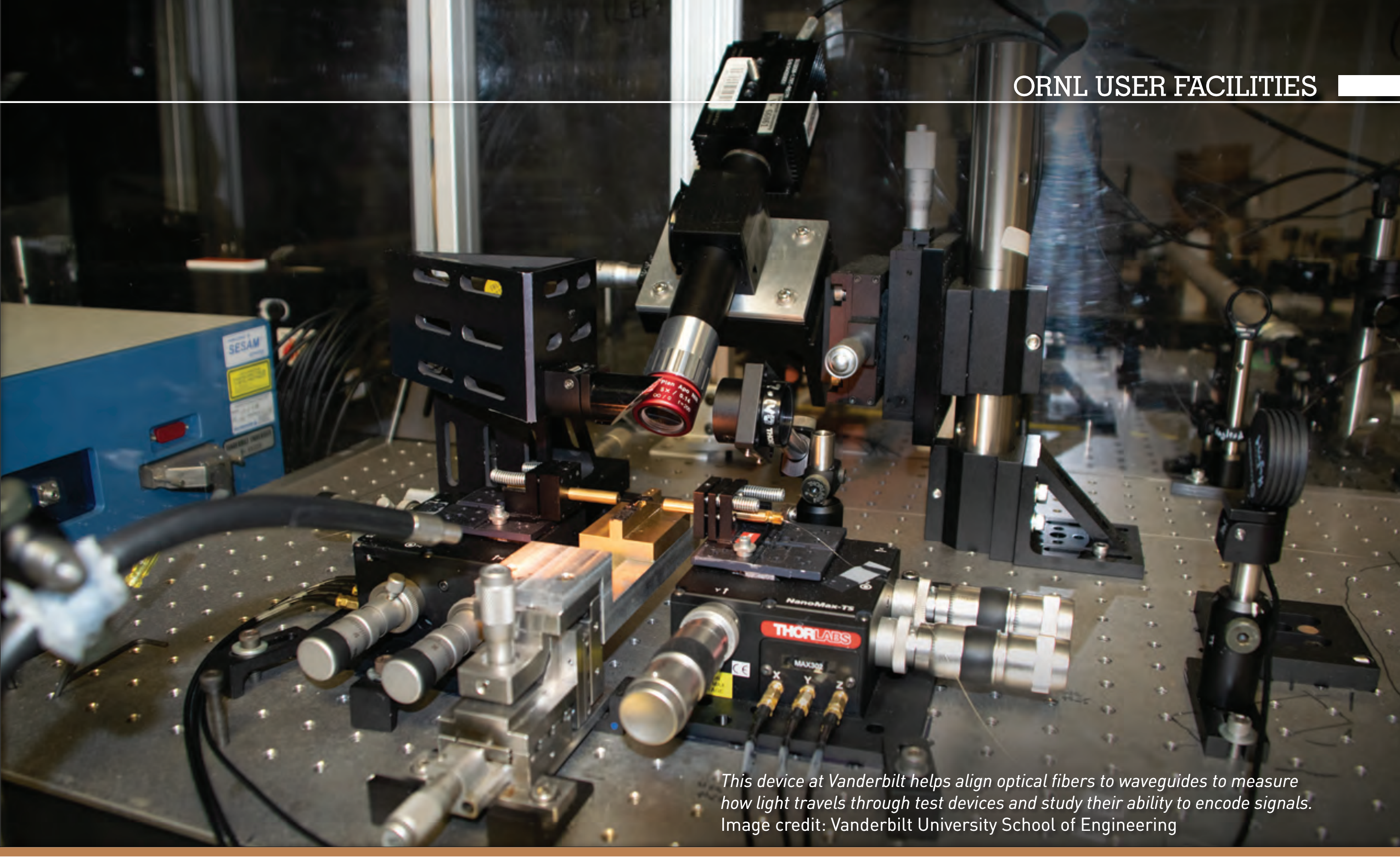
A third user facility for basic science at ORNL is the Center for Nanophase Materials Sciences. CNMS provides users with a wide range of specialized tools for imaging, synthesis, characterization and fabrication of novel nanoscale materials and assemblies, including the integration of hard and soft materials. These tools include optical and laser spectroscopy instruments, scanning probe microscopes, soft-matter transmission electron microscopes, scanning transmission electron microscopes, and helium-ion and atom-probe electron tomography instruments. A Class 1000 cleanroom environment facilitates controlled synthesis and directed assembly of nanomaterials.

> "*My research involved using electron beam lithography at the CNMS to create extremely small photonic structures. This included creating microscopic and nanoscopic waveguide devices on a chip that uses light, or photons, to transmit data as opposed to the electrons used by conventional computer chips.*
>
> — Vanderbilt University researcher **Sami Halimi**

Like all ORNL user facilities, CNMS, SNS and HFIR offer the national and international user community access to staff expertise, facilities and capabilities based on peer-reviewed proposals. Users submit their research proposals for review by independent scientists to ensure the most promising experiments are chosen. Scientists whose proposals are selected can conduct their research at no cost to them or to their institutions and companies, as long as they publish their results.



Vanderbilt University researcher Sami Halimi performs optical alignment for an ultrafast laser spectroscopy experiment to test silicon waveguide-based devices fabricated at the CNMS. Image credit: Vanderbilt University School of Engineering



This device at Vanderbilt helps align optical fibers to waveguides to measure how light travels through test devices and study their ability to encode signals.
Image credit: Vanderbilt University School of Engineering

CNMS also acts as a gateway for the nanoscience community to benefit from ORNL's neutron sources and computational resources. The user facility typically hosts over 600 unique users per year, with about 50 percent coming from American universities. Depending on the scope of work, users conduct research at CNMS lasting from as little as a few days to as much as several months—with some long-term projects even spanning years.

One user, Vanderbilt University researcher Sami Halimi, recently obtained his Ph.D. based on basic science experiments he conducted in large part at CNMS. He works in Professor of Electrical Engineering Sharon Weiss' research group at the university, about a 2.5-hour drive from ORNL.

"My research involved using electron beam lithography at the CNMS to create extremely small photonic structures," Halimi said. "This included creating microscopic and nanoscopic waveguide devices on a chip that uses light, or photons, to transmit data as opposed to the electrons used by conventional computer chips."

He added, "Vanderbilt's Weiss research lab has a long-standing relationship with the CNMS, and this has helped maintain excellent continuity for our students performing research there. Newer students benefit from the experience passed along by the more senior ones, so they don't need to start from scratch having CNMS staff teach them how to use the instruments and equipment."

Halimi described how continuity of student expertise and experience offers benefits beyond current research projects. "A lot of schools that don't have access to federally funded user facilities like we do tend to teach curricula focused on simulations, whereas students here can do the same types of modeling and then also conduct hands-on experiments at ORNL to validate those simulations."

Business and industry also benefit from access to ORNL's basic user facilities. This effect can be seen at DOE user facilities around the nation, where companies often locate nearby to have ready access to the research centers. The result is a mutually beneficial relationship as these firms help grow the local economies by directly and indirectly creating jobs and enlarging the tax base.

Finally, one of the most important benefits of ORNL's user facilities is that they play a large role in helping train future generations of scientists.

"When my students are arranging experiments at ORNL, they are responsible for contacting the user office, doing the paperwork, coordinating with the instrument scientists and facility staff, and handling many other details that help them learn soft skills, including people skills," Mourigal said. "This ties into the nation's National Quantum Initiative, designed, in part, to facilitate training our nation's future quantum workforce — because when we use neutrons, we often deal with complex quantum systems."

Mourigal explained that these basic science skills will not only benefit the collective U.S. scientific community but can also serve individual students well after they graduate and enter the workforce outside of academia.

"By providing students with neutron scattering expertise, I believe we are training tomorrow's high-level scientists, engineers and citizens to succeed in overcoming the nation's and world's many challenges that lie ahead."

OLCF: Serving up bleeding-edge compute power and expertise to the world's scientists

by Coury Turczyn
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While ORNL's Oak Ridge Leadership Computing Facility often makes headlines for hosting the world's fastest supercomputers, its ultimate achievement is more complex: helping researchers solve some of the world's most challenging scientific problems.

By offering scientists both world-class high-performance computing and world-leading expertise in scientific computing, the OLCF is a rare asset among DOE's array of institutions — with only the Argonne Leadership Computing Facility offering similar services.

The OLCF's primary systems are the 200-petaflop Summit — able to perform 200 million billion calculations every second — and the exascale-class Frontier — which will soon be available to users and is capable of more than a billion billion calculations each second. They attract scientists from around the world for open science projects that tackle the most computationally complex problems, from diverse scientific domains such as materials sciences, Earth sciences, astrophysics and biology. And with its quantum computing program, the OLCF also offers researchers a sneak peek into the future of scientific discovery.

Summit

Since its launch in 2018, the Summit supercomputer has been a world leader in not only computational power but also in scientific achievement. To date, the IBM AC922 system has served up over 113 million hours of computing time. Even with the advent of faster computers such as Frontier, Summit should prove invaluable for years to come.

Most users for OLCF systems are selected through highly competitive programs administered by DOE, primarily the annual Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, program, run by DOE's Office of Science. These awards pursue transformational advances in science and engineering and account for 60 percent of the available time on the leadership-class supercomputers at the OLCF and ALCF.

"INCITE allocations really serve as a bellwether for the next frontiers in advanced computing. The current class features a diverse portfolio of ambitious research campaigns representing

> "INCITE allocations really serve as a bellwether for the next frontiers in advanced computing. The current class features a diverse portfolio of ambitious research campaigns representing the most advanced techniques in high-performance computing in support of a broad range of both applied and basic research.
>
> — National Center for Computational Sciences Director **Gina Tourassi**

the most advanced techniques in HPC in support of a broad range of both applied and basic research," said Gina Tourassi, director of the National Center for Computational Sciences, which houses the OLCF. "We are proud to provide full-scale access to the world's most powerful systems to our users at the leading edge in their science domains."

> "To me, Summit is a step change. Its compute power is something I did not expect. Even the biggest calculations that we thought we were going to run would fit on 20 nodes of Summit — and Summit is over 4,000 nodes. So we really had to increase our ambition once we got access to the machine. I think that sort of step change requires you to rethink how you do your simulations and what simulations can actually be done. We changed our algorithmic frameworks, we changed our codes, we even changed how we answer the questions.
>
> — University of Michigan aerospace engineering professor **Venkat Raman**

Meanwhile, DOE's Office of Advanced Scientific Computing Research conducts the annual ASCR Leadership Computing Challenge. It grants one-year allotments of computing time to scientists from industry, academia and national laboratories whose work advances scientific and technological research in DOE mission areas such as fusion energy, geosciences, high energy physics and materials sciences.

Among its many success stories is a groundbreaking project led by University of Michigan aerospace engineering professor Venkat Raman to develop a rotating detonation engine, which detonates its fuel to create a wave front that continuously rotates

See OLCF: SERVING UP BLEEDING-EDGE COMPUTE POWER, page 20

OLCF: SERVING UP BLEEDING-EDGE COMPUTE POWER, page 19

within a cylindrical combustor. Many aerospace companies and governments around the world are pursuing this technology as well, but access to Summit has proved to be a critical advantage for his project, Raman said.

"To me, Summit is a step change. Its compute power is something I did not expect. Even the biggest calculations that we thought we were going to run would fit on 20 nodes of Summit — and Summit is over 4,000 nodes. So we really had to increase our ambition once we got access to the machine," Raman said. "I think that sort of step change requires you to rethink how you do your simulations and what simulations can actually be done. We changed our algorithmic frameworks, we changed our codes, we even changed how we answer the questions."

Quantum computing

Administered by the OLCF, the Quantum Computing User Program, or QCUP, awards time on quantum computers owned by companies such as IBM, Quantinuum (formerly Honeywell) and Rigetti Computing to scientists with quantum-specific projects. Although the systems are not in-house, OLCF administrators benefit by getting first-hand experience at managing open science projects on cutting-edge quantum computers.

"As a facility, we're trying to understand when quantum computing as a technology will be ready for prime time," said ORNL's Travis Humble, manager of the user program and interim director of the Quantum Science Center. "At the moment, it's very experimental, with a focus on exploration and discovery. We established the user program to monitor the technology and track the progress that the users are making."

The 4-year-old program has supported over 100 users running more than 70 projects by providing compute time from a variety of companies that are producing quantum computers.

"One of the things that differentiates QCUP is that we're not advocating for a particular quantum computing system. We're very agnostic to the individual devices," Humble said. "We really just want people to do the best science."

Fengqi You, the Roxanne E. and Michael J. Zak Professor in Energy Systems Engineering in Cornell University's College of Engineering, used the program to successfully test a proposed quantum computer-based artificial intelligence system for identifying and diagnosing faults in electrical power grids. Being able to access an actual quantum computer from D-Wave Systems through QCUP has been a big boost to designing his new detection system.

"Quantum computers can help improve certain aspects of the training methodology by providing better gradient estimates

> "*Exascale computing gives us tremendous opportunities to make scientific advancements in plasma physics that were utterly beyond our reach before. Also, it allows us to do more simulations. So instead of doing a single simulation once, we can play with the problem and find out which physics conditions work best. For tumor therapy this means we can discover new, innovative ways to improve the energy, quality and precision of proton beams.*
>
> — University of Delaware associate professor **Sunita Chandrasekaran**

The University of Delaware's Sunita Chandrasekaran (facing camera) is developing an open-source simulations framework for plasma and laser-plasma physics. Also pictured are, from left, Thomas Huber, Michael Carr and Kristina Holsapple. Image credit: University of Delaware

compared to their classical counterparts, thus improving convergence and resulting in better generalization," You said. "Apart from the improvement in training techniques, the proposed fault diagnosis framework also demonstrates faster response times than popular fault detection methods."

Frontier

After years of planning and construction, the world's most powerful supercomputer — Frontier — brings an eightfold increase in computational power over Summit, allowing researchers to tackle more extensive problems and answer more complex questions than ever before.

Early access to Frontier and its test platforms were granted through the OLCF's Center for Accelerated Application Readiness program, or CAAR. Through the program, the OLCF partners with application core developers, vendor partners, and OLCF staff members to optimize scientific applications for exascale performance, ensuring that Frontier will perform large-scale science on day one of full user operations. To be selected for the CAAR program, projects had to show a high potential for scientific advancement that could be achieved on petascale computers like Summit.

Eight CAAR projects were chosen for Frontier, with simulations ranging in scale from protons to our galaxy.

"Exascale computing gives us tremendous opportunities to make scientific advancements in plasma physics that were utterly beyond our reach before," said Sunita Chandrasekaran, an associate professor at the University of Delaware who is developing an open-source simulations framework for plasma and laser-plasma physics with applications in radiation therapy, high-energy physics, and photon science. "Also, it allows us to do more simulations. So instead of doing a single simulation once, we can play with the problem and find out which physics conditions work best. For tumor therapy this means we can discover new, innovative ways to improve the energy, quality and precision of proton beams."

Evan Schneider, an assistant professor at the University of Pittsburgh, has been developing her Cholla astrophysics simulation code on a variety of different systems over the years — but Frontier is a "galaxy-changer," offering unprecedented resolution.

"Using our Cholla astrophysics software on an exascale machine, we will be able to run a simulation where we can directly resolve what's happening in small patches of the galaxy," Schneider said. "So instead of having to make assumptions about how the stars are forming and how the supernovae are affecting the galaxy, we can actually just directly simulate that using the physics that we understand. There's no other computer that's big enough and has enough computing power to get the resolution that we require."

National user facilities

use applied science to accelerate industry growth

by Jennifer Burke
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When U.S. industries need to research, test, troubleshoot and perfect an innovation before it reaches the marketplace, many turn to DOE's applied science user facilities at ORNL.

Sponsored by DOE's Office of Energy Efficiency and Renewable Energy, the Manufacturing Demonstration Facility, Carbon Fiber Technology Facility, Building Technologies Research and Integration Center, and National Transportation Research Center provide private industry as well as universities and other laboratories access to the capabilities and expertise necessary to quickly move new technologies from research and demonstration to deployment in support of national priorities such as decarbonization.

> *"What makes a facility like the Manufacturing Demonstration Facility, or MDF, unique is that we colocate our scientists and support staff with users, which allows them to work together while accessing multiple disciplines all integrated under one roof.*
>
> — ORNL Energy Science and Technology Directorate Associate Laboratory Director **Xin Sun**

These facilities foster place-based innovation, applying ORNL's resources to address community needs, fuel regional innovation hubs and spur economic development and job growth. Industries partner with user facilities through technical collaborations and cooperative R&D agreements, or CRADAs.

To date, these facilities have enabled more than 140 patented technologies and collaborated with more than 700 industrial partners, universities and laboratories.

Many of these technologies have been licensed by some of the nation's largest companies, including GE, Cummins, ExOne and Zeiss. Small and newly established companies also work with the user facilities, collaborating on-site and alongside ORNL researchers.

Economic impact

"What makes a facility like the Manufacturing Demonstration Facility, or MDF, unique is that we colocate our scientists and support staff with users, which allows them to work together while accessing multiple disciplines all integrated under one roof," said Xin Sun, associate laboratory director for ORNL's Energy Science and Technology Directorate..

Sun said this type of model not only gets products to the marketplace faster, but also trains, educates and guides workforce development and enables next-generation technologies.

"We form strategic partnerships with equipment managers, for example, so that we can have national impact," she added. "The MDF's partnerships alone have had about a billion-dollar impact on U.S. manufacturing and enabled many startups."

In 2018, when Knoxville, Tennessee-based entrepreneur Jonaaron Jones opened Volunteer Aerospace's headquarters in the Hardin Valley area about a 15-minute drive from ORNL's main campus, he made sure the growing company was located near the MDF.

Jones worked with the facility while he was an MDF research engineer, investigating the use of a powder bed additive manufacturing process to produce parts and products for the aerospace and defense industries. He spent four years fine-tuning that process and says the MDF served as an incubator for his company.

In just under three years, Jones was able to grow the company to seven employees, adding five additive systems capable of fabricating components. One of the first machines Volunteer Aerospace began working with was the original Concept Laser, a machine that Jones became familiar with while at the MDF. He noted that having access to ORNL research expertise enabled his company's rapid expansion, something that would not have been possible without the support of the MDF. Volunteer Aerospace's growth ultimately led to a company acquisition in late 2021 by Florida-based additive solutions provider Beehive 3D, Inc.

Meeting the challenge

Making the seemingly impossible a reality is what researchers at these user facilities thrive on. Early in the COVID-19 pandemic in 2020, researchers from the MDF collaborated with ORNL's Carbon Fiber Technology Facility, or CFTF, and industry partner Cummins on ways to produce filter media for N95 masks.

Merlin Theodore, ORNL's Advanced Fibers Manufacturing Group leader, converted the CFTF's melt blowing capability to the production of polypropylene. Polypropylene is a nonwoven material that is permanently electrostatically charged, with millions of microfibers layered on top of each other to filter out virus particles smaller than a millionth of a meter.

Theodore transferred the capability to Cummins, an engine and power generation manufacturer, so that the company could convert its own melt blowing line into producing N95 filter material. The company ultimately made enough filter media to supply a million masks a day.

"We knew melt blowing, but we could not have gotten up to speed without the interactions with ORNL," said Christopher Holm, Cummins' director of filter media technology. "Their technical guidance helped us become operational in a short amount of time so that we could meet the demand and supply our customers with material during a time of crisis."

Said Theodore: "Our goal is to transfer our technology to industry partners to increase U.S. competitiveness in manufacturing. This also supplies a critical need for our country, creates job growth and stimulates the economy. We are the catalyst that helps industry bring technology to the consumer."

As the pandemic progressed and COVID-19 vaccines became available, Carrier Global Corporation needed to figure out how to keep them properly stored and refrigerated when being trans-

See NATIONAL USER FACILITIES USE APPLIED SCIENCE, page 24

ORNL researchers Diana Hun, left, and Brenda Smith conduct a leak detection experiment in the Building Technologies Research and Integration Center. Image credit: ORNL

NATIONAL USER FACILITIES USE APPLIED SCIENCE, page 23

ported to rural and remote areas. To solve the challenge, the refrigerant manufacturing expert consulted with researchers within DOE's Building Technologies Research and Integration Center, or BTRIC, at ORNL.

Carrier and ORNL retrofitted a commercial storage container on the BTRIC campus, where they conducted experiments to determine the lowest temperature that could be maintained for the longest period. Six months of testing determined that an all-electric unit container could provide precise temperature control at the minus-30-to-35-degree range necessary for COVID-19 vaccines. By optimizing package placements within the container to hold 20 polystyrene foam packages, each with around 5,000 doses, one container could transport 100,000 refrigerated doses of vaccine.

"By collaborating with BTRIC at ORNL, we have been able to validate our mobile cold storage solution that can support COVID-19 vaccine distribution," said Nader Awwad, Carrier's director of engineering.

> *"ExxonMobil came to ORNL because we know fuels and emissions, and we know engines. The NTRC user facility allowed Exxon to perform controlled engine-based experiments, filling the gap between bench-scale and full-engine tests. This one collaboration helped develop Exxon's whole research strategy for the development of next-generation lubricants.*
>
> — ORNL's Buildings and Transportation Science Division Director **Robert Wagner**

"This project is an example of how the scientific creativity and resources of a national user facility and coordination with industry can lead to meeting the needs of our nation during a critical period," said Melissa Lapsa, ORNL's building technologies program manager. "Our researchers recognized the urgency of Carrier's need and brought the appropriate resources together so that we could quickly deliver solutions."

Powerful collaboration

Working with industry leaders like Carrier is part of the day-to-day operations of the national user facilities. In recent years, the National Transportation Research Center, or NTRC, partnered with another global brand, ExxonMobil, to operate a one-of-a-kind experimental engine that would enable the development of next-generation lubricants for the marine industry.

Exxon installed a custom-built, one-tenth-scale marine diesel engine called the Enterprise at the NTRC. At 12 feet tall and weighing more than 16,000 pounds, the flexible-fuel, single-cylinder engine has a rated speed of 625 rpm to match the speed of a full-scale engine. Overall, the ORNL and Exxon collaboration informed the production of a new suite of low-sulfur fuels, known as EMF.5, that adhere to sulfur-compliant marine fuel specifications.

"ExxonMobil came to ORNL because we know fuels and emissions, and we know engines," said Robert Wagner, director of ORNL's Buildings and Transportation Science Division. "The NTRC user facility allowed Exxon to perform controlled engine-based experiments, filling the gap between bench-scale and full-engine tests. This one collaboration helped develop Exxon's whole research strategy for the development of next-generation lubricants."

"This engine is a dream come true," said John Fogarty, research team lead for ExxonMobil. "We wanted to put our engine here to have the expertise Oak Ridge provided."

Industry partnerships also feed an innovation ecosystem — something that is uniquely suited to national user facilities. More than 5,000 companies have visited MDF alone, resulting in more than 180 collaborative research projects. Each collaboration helps shape a future vision for U.S. industry based on the problems and needs discovered through core scientific research and development. Ultimately, innovation cultivated within a user facility can lead to workforce development initiatives, not only creating jobs but also helping to shape the next generation of innovators.

Within advanced manufacturing, specifically, Sun noted that the MDF aims to develop technology faster than the competition can copy.

"We have close to a hundred manufacturing systems installed at the MDF, and these all support the production of energy-efficient products with benefits extending across the nation's economy. We're creating and driving a system of innovation," she said.

Emma Betters, left, an ORNL machine tooling researcher, leads the assembly of an electrostatic charging device for N95 filter material at the Manufacturing Demonstration Facility. Image credit: Carlos Jones, ORNL

The secret lives of corn plants caught 'on camera'

by Paul Boisvert
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Corn is a seemingly simple plant, but underground it has a very complicated life.

Despite decades of scientific studies and biosphere modeling, researchers have been largely unable to quantify how water and soil nutrients pass into plant roots at microscopic scales. This is why details on the dynamic functions of roots are mostly absent from terrestrial biosphere models or are greatly simplified.

Yet, root activity is highly variable and has substantial impacts on soil properties, including water retention, water flow rate, and the uptake of nutrients, chemicals and pollutants in the ground. Capturing root dynamics and their impacts on soil moisture in 3D and in real time would allow a better representation of roots for modeling purposes.

To make it easier to study and understand root activity in situ, ORNL scientists at the High Flux Isotope Reactor have developed new methods of neutron imaging. Neutrons are highly penetrating and nondestructive, properties that enable them to scan roots through sandy soil. When used in combination with novel computer algorithms, neutrons enabled researchers to capture computed tomography images of roots faster than conventional methods, allowing more accurate assessment of real-time root activity.

"Neutron computed tomography, or CT, uses neutrons to look inside objects without slicing them open, similar to the X-ray CT scans used in medical applications," said Jeff Warren, senior staff scientist for ORNL's Environmental Sciences Division. "Directly applying conventional CT methods to image

ORNL used neutron CT scanning at HFIR and an algorithm to study root dynamics in 3D and real time. Image credit: Genevieve Martin, ORNL

objects that are changing during a scan can be extremely challenging. That's why we are developing algorithms that collect data much more quickly, along with algorithms to capture complete images of root dynamics, something that will help further research to reduce uncertainty in future terrestrial biosphere models."

Direct physical sampling of soil, water and roots can damage a plant's tissue and the area around its roots, leading to the collection of incomplete or inaccurate root function data. The algorithms being developed at ORNL are powerful enough to accurately reconstruct the functions in real time.

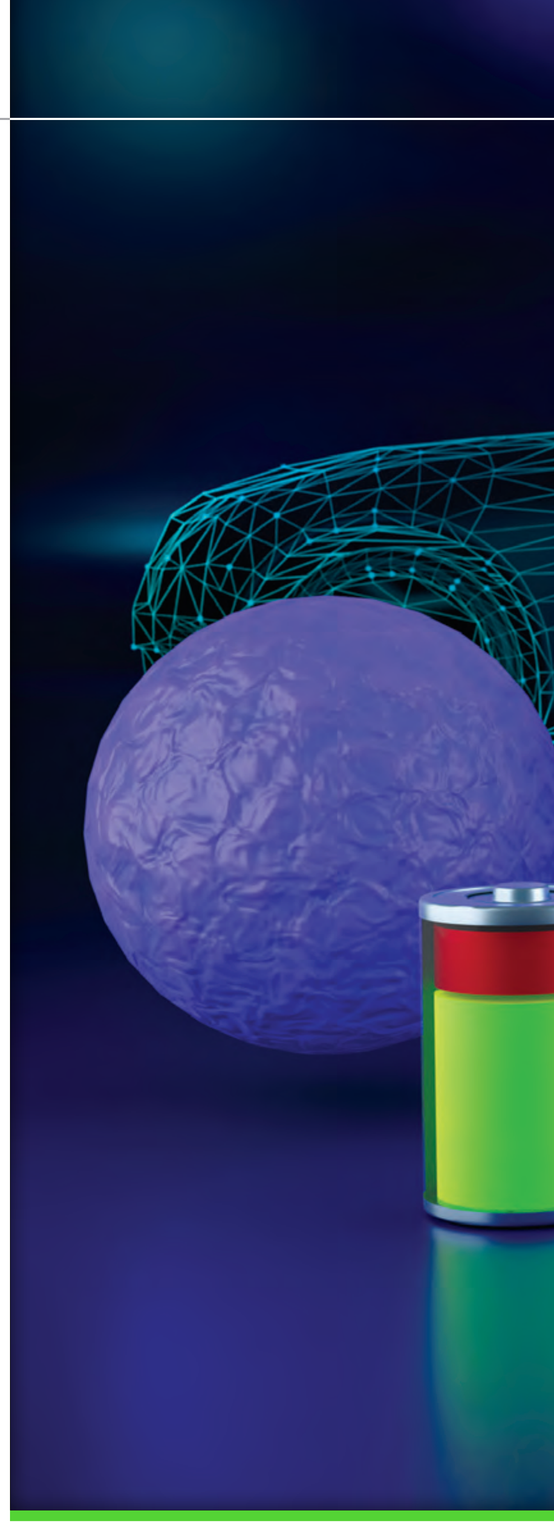
"Using artificial intelligence–based algorithms to help obtain high-fidelity images is becoming more and more popular in the field of CT," said Singanallur "Venkat" Venkatakrishnan, research staff scientist in ORNL's Electrification and Energy Infrastructure Division. "We are training machine learning models to produce higher-quality images of root structures and root activity from extremely complex CT data in a fraction of the time typically required by other methods."

At the HFIR imaging beamline, the team injected water into quartz cylinders filled with a sand–clay soil mix to assess the 3D dynamics of water uptake in corn plant roots.

"One of our goals was to visualize in 3D how fast water moves through the soil and is taken up into the roots, which previously was limited to visualizing 2D images of roots compressed between thin plates," Warren said. "The neutron imaging facility at HFIR helped us observe and record the uptake process in exposures from 0.1 to 10 seconds long to capture the water uptake in near real time instead of as just individual snapshots. Neutron CT could eventually be used to capture entire root scans in less than 90 seconds."

The new faster experiments produced more than 2 terabytes of data and over 160,000 high-resolution images. CT reconstructions from the data will be compared against independent soil water flow models to validate and refine the representations of 3D water flow between soils and roots. Results can be used to inform the development of more advanced terrestrial biosphere models that include soil hydraulics — a current priority for the DOE Office of Science.

ORNL helps Nobel laureate improve battery cathodes



by Paul Boisvert
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In the late 1970s, M. Stanley Whittingham was the first to describe the concept of rechargeable lithium-ion batteries, an achievement for which he would share the 2019 Nobel Prize in Chemistry. Yet even he couldn't have anticipated the complex materials science challenges that would arise as these batteries came to power the world's portable electronics.

One persistent technical problem is that every time a new lithium-ion battery is installed in a device, up to about one-fifth of its capacity is lost before the device can be recharged the very first time. That's true whether the battery is installed in a laptop, camera, wristwatch or electric vehicle.

The cause is impurities that form on the nickel-rich cathodes — the positive side of a battery through which its stored energy is discharged.

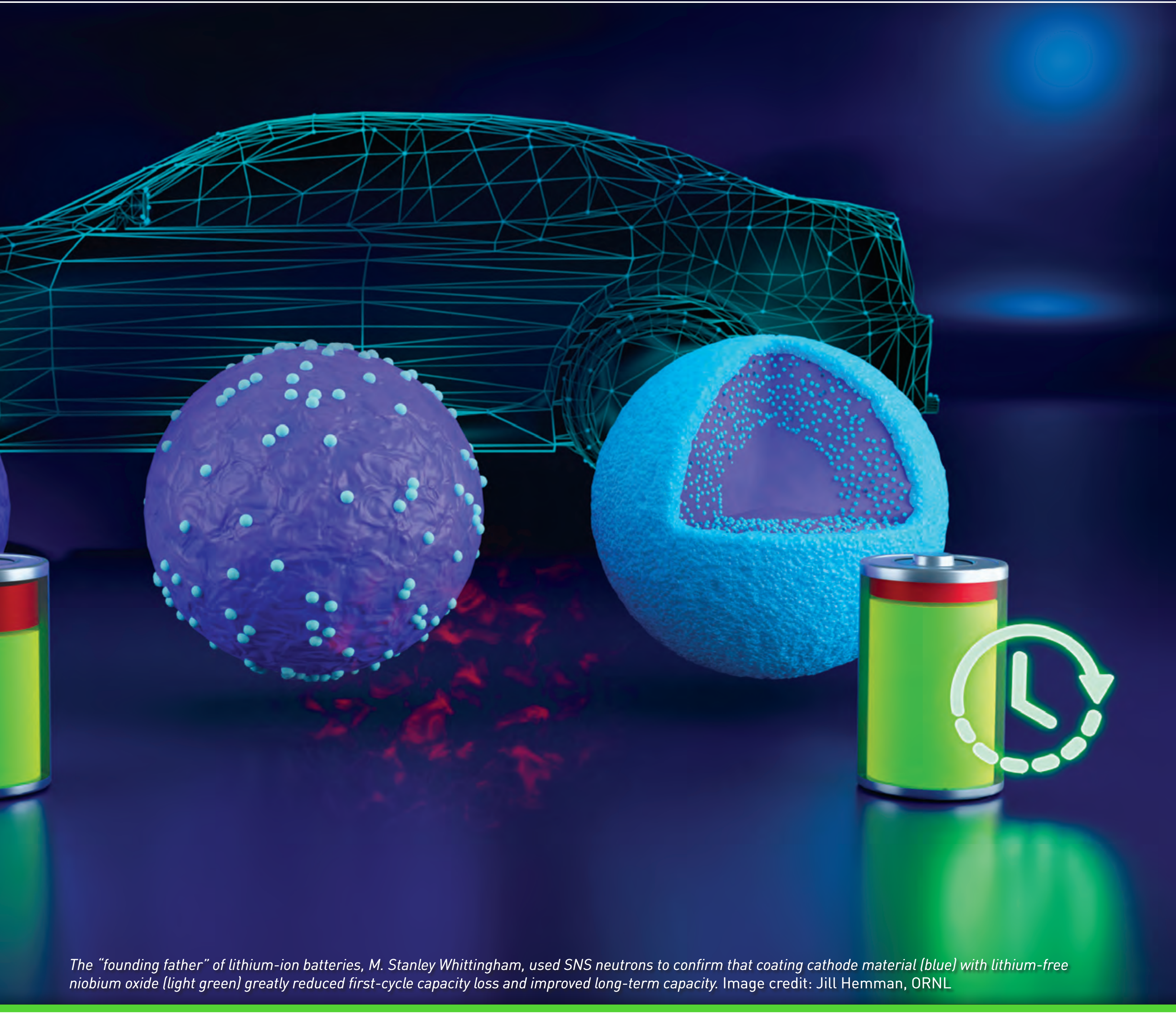
To find a way of retaining the lost capacity, Whittingham led a group of researchers using X-rays and neutron scattering at ORNL's Spallation Neutron Source to test whether treating a leading cathode material — a layered nickel-manganese-cobalt material called NMC 811 — with a lithium-free niobium oxide would lead to a longer-lasting battery.

"We correctly predicted the lithium-free niobium oxide would form a coating that allows lithium ions to penetrate into the cathode," said Whittingham, now a State University of New York distinguished professor and director of the NorthEast Center for Chemical Energy Storage, a DOE Energy Frontier Research Center.

Lithium batteries have cathodes made of alternating layers of lithium and nickel-rich oxide materials — chemical compounds containing at least one oxygen atom — because nickel is relatively inexpensive and helps deliver higher energy density and greater storage capacity at a lower cost than other metals.

But the nickel in cathodes is relatively unstable and therefore reacts easily with other elements, leaving the cathode surface covered in undesirable impurities that reduce the battery's storage capacity by 10 to 18 percent during its first charge–discharge cycle. Nickel can also cause instability inside the cathode, which further reduces storage capacity over extended periods of charging and discharging.

To understand how niobium affects nickel-rich cathode materials, the scientists performed neutron powder diffraction studies using the VULCAN engineering materials diffractometer at SNS. They measured the neutron diffraction patterns of pure NMC 811 and niobium-modified samples.



The "founding father" of lithium-ion batteries, M. Stanley Whittingham, used SNS neutrons to confirm that coating cathode material (blue) with lithium-free niobium oxide (light green) greatly reduced first-cycle capacity loss and improved long-term capacity. Image credit: Jill Hemman, ORNL

"Neutrons easily penetrated the cathode material to reveal where the niobium and lithium atoms were located, which showed how the niobium modification process works," said Hui Zhou, battery facility manager at NECCES.

"The neutron scattering data suggests the niobium atoms stabilize the surface to reduce first-cycle loss, while at higher temperatures the niobium atoms displace some of the manganese atoms deeper inside the cathode material to improve long-term capacity retention."

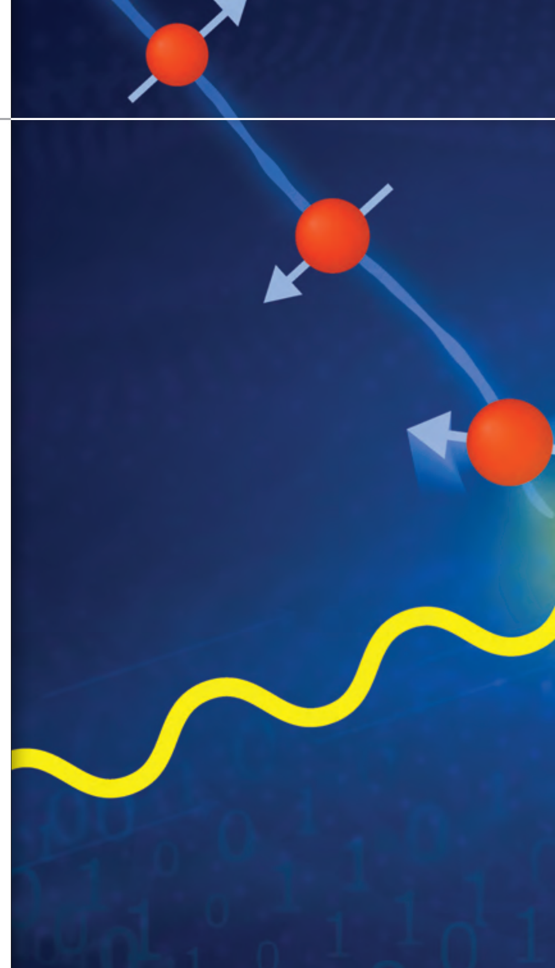
The results of the experiment showed a reduction in first-cycle capacity loss and an improved long-term capacity retention of greater than 93 percent over 250 charge–discharge cycles.

"The improvements make niobium-modified NMC 811 a candidate material for use in higher energy density applications, such as electric vehicles," said Whittingham. "Combining a niobium coating with the substitution of niobium atoms for manganese atoms may be a better way to increase both initial capacity and long-term capacity retention. These modifications can be easily scaled up."

Whittingham added that the research supports the objectives of the Battery500 Consortium, a multi-institution program of the DOE Office of Energy Efficiency and Renewable Energy. The program is working to develop next-generation lithium-metal battery cells delivering up to 500 watt-hours per kilogram versus the current average of about 220 watt-hours per kilogram.

Key witness

spills secrets of 'spooky' quantum entanglement



A material's spins, shown as red spheres, are probed by scattered neutrons. Applying an entanglement witness, such as the QFI calculation pictured, causes the neutrons to form a kind of quantum gauge capable of distinguishing between classical and quantum spin fluctuations. Image credit: Nathan Armistead, ORNL

by Elizabeth Rosenthal
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Nearly 90 years after Albert Einstein famously coined the phrase "spooky action at a distance" to describe quantum entanglement, an ORNL-led team demonstrated a technique capable of proving the presence of entanglement, or communication without a physical connection, between magnetic particles, or spins, in a quantum material.

The technique uses inelastic neutron scattering to measure an entity known as quantum Fisher information, or QFI. QFI is part of a class of measurable quantities called quantum entanglement witnesses, which keep track of spins that cross the threshold between the classical and quantum realms.

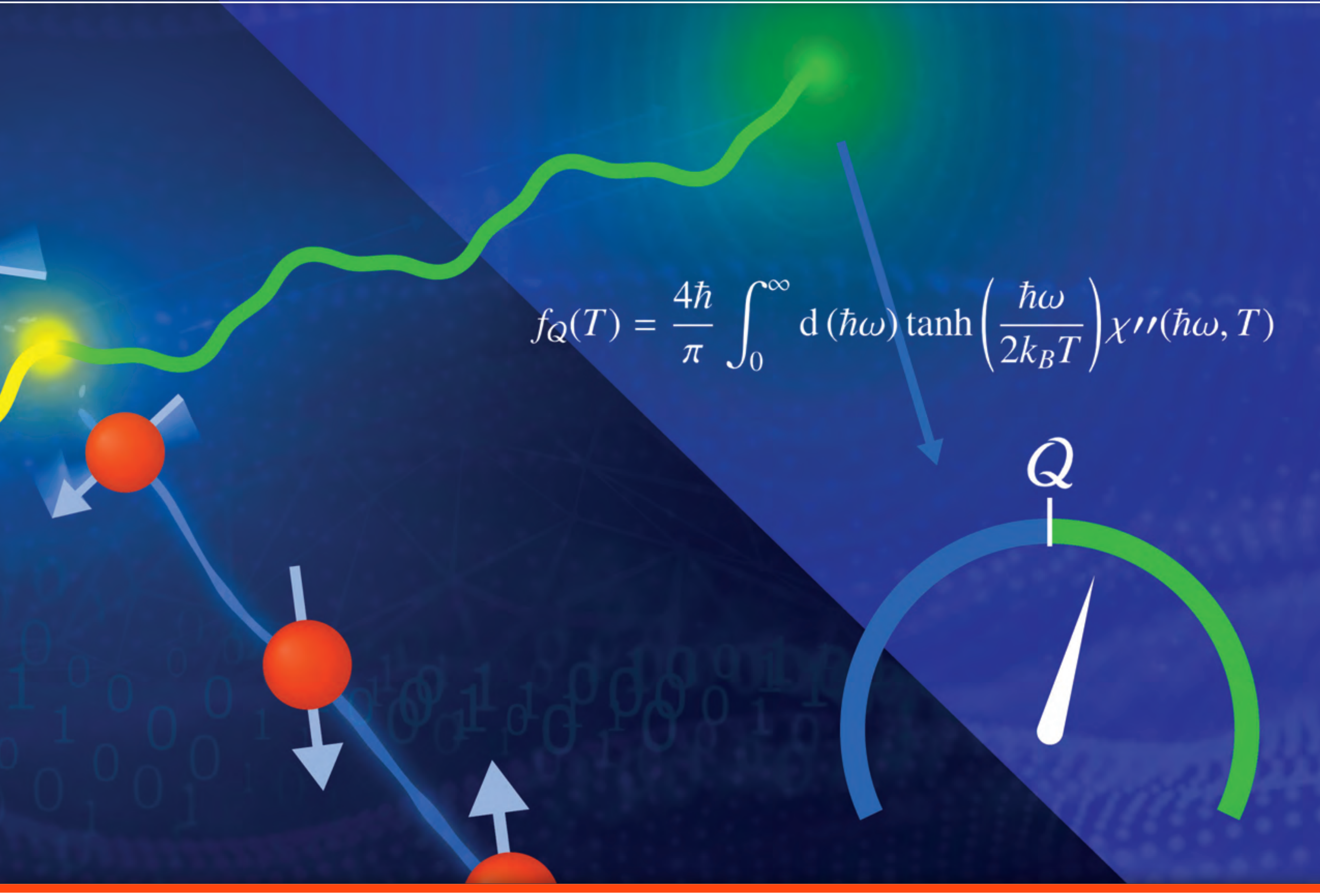
> "The QFI witness showed a close overlap between theory and experiment, which makes it a robust and reliable way to quantify entanglement.
> — ORNL research associate **Allen Scheie**

Led by former ORNL scientist Alan Tennant, a professor at the University of Tennessee, Knoxville, a multi-institutional team conducted neutron scattering experiments and computational simulations to analyze QFI and two other witnesses. This team included researchers from ORNL, Helmholtz Zentrum Berlin, the Technical University of Berlin, Institut Laue-Langevin in France, Oxford University and Adam Mickiewicz University in Poland.

To ensure that the witnesses could be trusted, the team applied them to a material they knew was entangled. All three detected large collections of entangled spins, but QFI fared especially well.

"The QFI witness showed a close overlap between theory and experiment, which makes it a robust and reliable way to quantify entanglement," said Allen Scheie, a postdoctoral research associate at ORNL.

Entanglement witnesses have existed for decades, but earlier experiments typically detected one pair of particles at a time, which posed a problem for researchers hoping to apply these tools to



study solid materials composed of huge numbers of particles.

Having overcome the witnesses' previous limitations, the researchers can now use them to characterize solid materials and study exotic behavior in superconductors and quantum magnets. Cultivating a better understanding of these resources could reveal untapped potential for data storage and computing applications.

Random thermal motion, which occurs at any temperature above absolute zero, can cause fluctuations in a material that mimic quantum behavior. As a result, many modern methods cannot distinguish between these false alarms and actual quantum activity. The team's demonstration, the most comprehensive QFI study since the witness was first proposed six years ago, drew a distinct line between classical and quantum fluctuations.

"Using inelastic neutron scattering to quantify QFI offers a measure of quantum entanglement that doesn't depend on any particular theoretical model," said coauthor and ORNL Corporate Fellow Steve Nagler.

Having established that QFI could consistently recognize entanglement, the team tested a second, more complex material. Applying a magnetic field triggered an entanglement transition, a phenomenon in which the amount of entanglement fell to zero before reappearing, giving the researchers new insights into that material.

To achieve these results, they studied both materials using neutron scattering and compared new data gleaned from experiments at ORNL's Spallation Neutron Source to legacy data collected from older experiments conducted at the ISIS Neutron Source in England and the Institut Laue-Langevin in France.

Finally, the team ran complementary simulations at ORNL to validate these findings against idealized theoretical data. These collaborations were facilitated by the Quantum Science Center, a DOE National Quantum Information Science Research Center headquartered at ORNL.

Neutrons are an ideal tool for probing the properties of a material because of their neutral charge and nondestructive nature.

"It's extremely difficult to measure and prove that entanglement is present, but neutrons allowed us to complete this necessary step," Scheie said.

The team's results answer quantum entanglement questions originally asked by the founders of quantum mechanics, and Scheie expects QFI calculations to become part of the standard procedure for neutron scattering experiments that aim to demystify even the most complicated quantum materials.

Real-world demonstration

leads to quantum networking milestone

by Elizabeth Rosenthal
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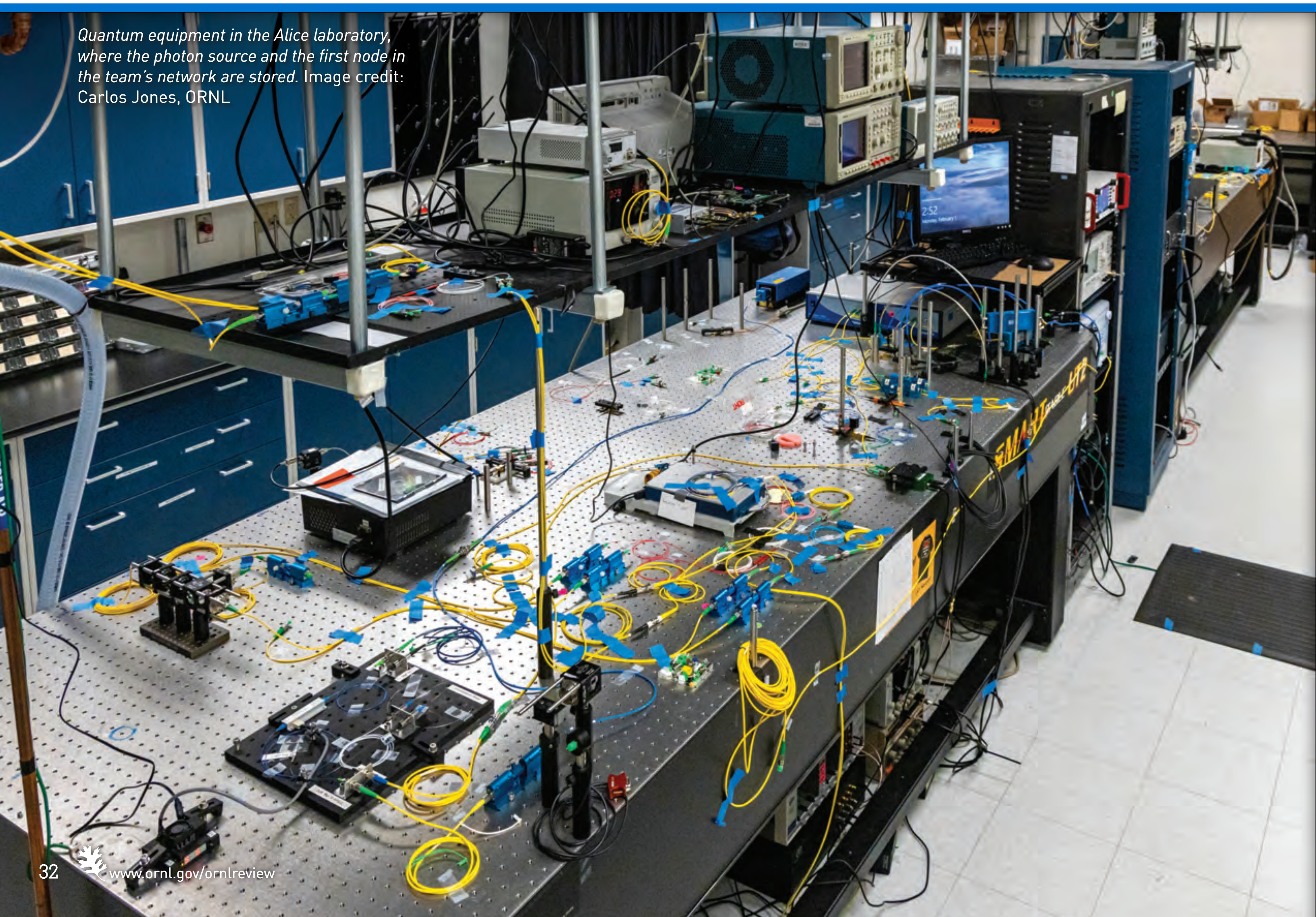
A team from ORNL, Stanford University and Purdue University have developed and demonstrated a novel, fully functional quantum local area network, or QLAN, that connects three buildings on ORNL's campus through existing communication channels made of optical fiber.

This flexible network allows researchers to make real-time adjustments to information shared among three remote nodes whimsically named Alice, Bob and Charlie using entangled photons. These paired particles of light exhibit strong correlations, regardless of the geographical distance between them.

Previously, QLANs had been implemented only in tabletop studies. By experimenting with the new network's adaptability at a larger scale, the researchers are helping lay the foundation for the highly anticipated quantum internet, which will consist of next-generation quantum computers and sensors.

"Our goal is to develop the fundamental building blocks we need to demonstrate quantum networking applications so that they can be deployed in real networks to realize quantum advantages," said Nicholas Peters, ORNL's Quantum Information Science section head.

The researchers demonstrated a quantum communications protocol called remote state preparation. This technique



Quantum equipment in the Alice laboratory, where the photon source and the first node in the team's network are stored. Image credit: Carlos Jones, ORNL involves taking precise measurements of one photon in an entangled pair, then communicating the results to the second photon so that a correlated quantum state is realized. Repeating this process enabled efficient quantum communication among all the paired links in the QLAN. They published this accomplishment, which had not previously been realized on any network, in the journal *PRX Quantum*.

The team also incorporated a quantum communications technique called flexible grid bandwidth provisioning, which allocates and reallocates quantum resources to network users without disconnecting the QLAN. This method provides some built-in fault tolerance that allows network operators to respond to an unanticipated event, such as a broken fiber, by rerouting traffic to other areas without disrupting the network's speed or security.

"Because the demand in a network might change over time or with different configurations, you don't want to have a system with fixed wavelength channels that always assigns particular users the same portions," said research scientist Joseph Lukens. "Instead, you want the flexibility to provide more or less bandwidth to users on the network according to their needs."

Nodes in a quantum network must be precisely synchronized to communicate effectively, so the team relied on GPS, the same versatile and cost-effective technology that uses satellite data to provide everyday navigation services. A shared signal from a GPS antenna ensured that GPS-based clocks in each laboratory remained synchronized within a few nanoseconds.

Having obtained timestamps for the arrival of entangled photons captured by photon detectors, the researchers sent measurements from the QLAN to a classical network, where they compiled high-quality data from the three campus buildings connected by the QLAN.

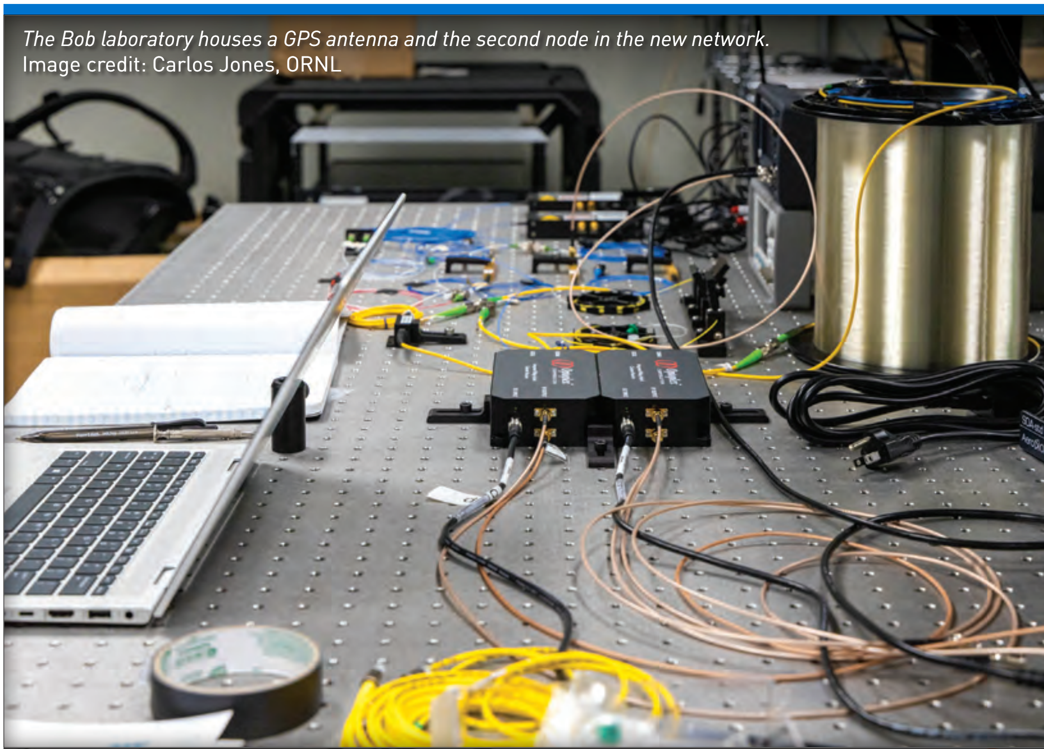
"This part of the project became a challenging classical networking experiment with very tight tolerances," Lukens said. "Timing on a classical network rarely requires that level of precision or that much attention to detail regarding the coding and synchronization between the different laboratories."

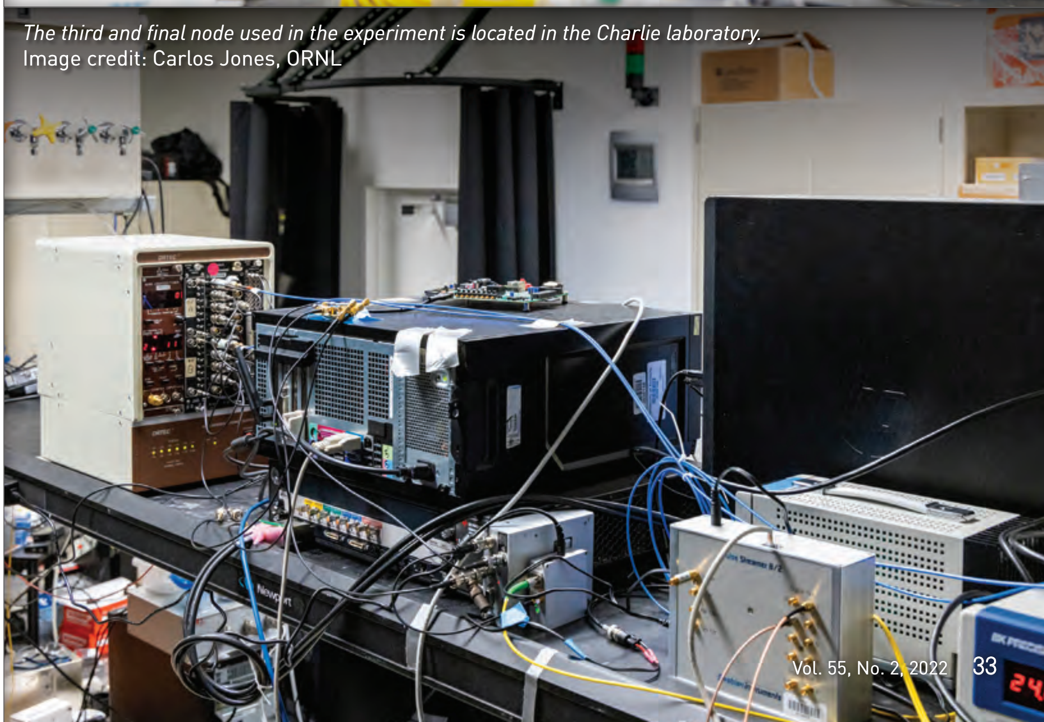
The researchers are fine-tuning the QLAN to support the eventual development of the quantum internet.

"The internet is a large network made up of many smaller networks," said Muneer Alshowkan, a research scientist in ORNL's QIS section. "The next big step toward the development of a quantum internet is to connect the QLAN to other quantum networks."

Results from these experiments could also inform improved detection techniques, such as those used to seek evidence of dark matter, the invisible substance thought to be the universe's predominant source of matter.

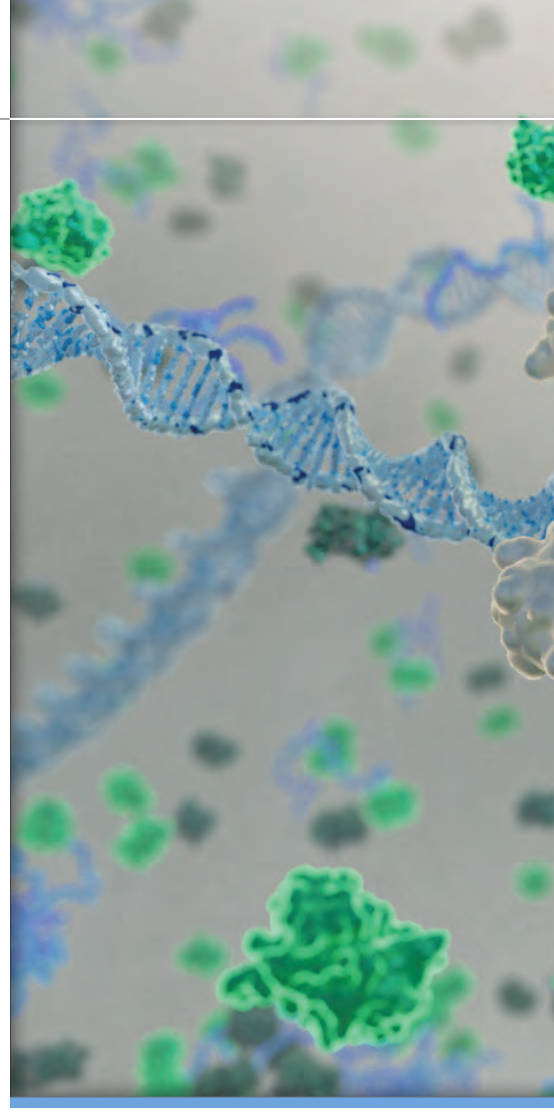
"By developing this technology, we aim to lower the sensitivity needed to measure those phenomena to assist in the ongoing search for dark matter and other efforts to better understand the universe," Peters said.


The Bob laboratory houses a GPS antenna and the second node in the new network.
Image credit: Carlos Jones, ORNL


The third and final node used in the experiment is located in the Charlie laboratory.
Image credit: Carlos Jones, ORNL

New biosensors

shine a light on CRISPR gene editing



by Kim Askey
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Detecting the activity of CRISPR gene editing tools in organisms with the naked eye and an ultraviolet flashlight is now possible using technology developed at ORNL. Scientists demonstrated these real-time detection tools in plants and anticipate their use in animals, bacteria and fungi with diverse applications for biotechnology, biosecurity, bioenergy and agriculture.

CRISPR technologies have quickly become the primary tools of bioengineering. Identifying whether an organism has been modified by CRISPR was previously a complex and time-consuming process.

> "Before this, the only way to tell if genome engineering occurred was to do a forensic analysis. To be successful, you would need to know what the genome looked like before it was rewritten. We wanted to design a platform where we could proactively observe CRISPR activity.
>
> — Secure Ecosystem Engineering and Design Science Focus Area head **Paul Abraham**

"Before this, the only way to tell if genome engineering occurred was to do a forensic analysis," said Paul Abraham, a bioanalytical chemist and head of ORNL's Secure Ecosystem Engineering and Design Science Focus Area. "To be successful, you would need to know what the genome looked like before it was rewritten. We wanted to design a platform where we could proactively observe CRISPR activity."

The research team developed an efficient self-detect solution that takes advantage of the way CRISPR works to trigger the technology to reveal itself.

Under normal conditions, CRISPR works by connecting with a short RNA sequence, known as the guide RNA, as it leads CRISPR to a matching DNA sequence. When the target DNA is found, CRISPR modifies the DNA by acting like tiny molecular scissors to cut through one or both strands of DNA, depending on the type of CRISPR technology in use.

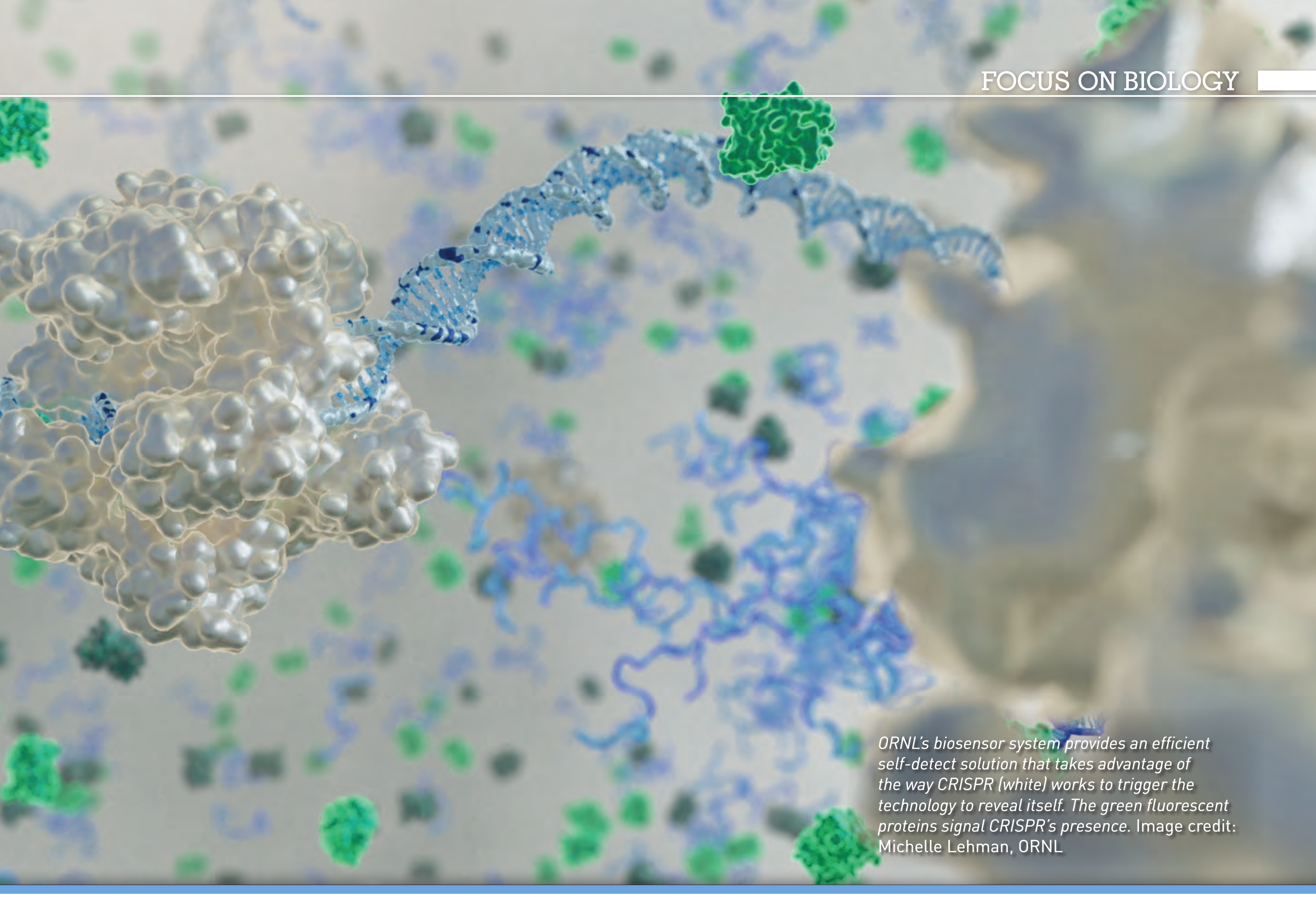
Abraham likens their method to an alarm system with two components: a biosensor guide RNA that redirects CRISPR activity and a reporter protein that flags the activity. Researchers encode the two components into an organism's DNA to enable the monitoring system.

With the self-detect system in place, the biosensor guide RNA intercepts CRISPR, preventing CRISPR from connecting with its original gene target and redirecting CRISPR to a specific DNA sequence that encodes for a nonfunctioning green fluorescent protein, or GFP. When CRISPR edits the sequence, it flips a switch that produces functioning GFP, which creates a green glow signaling CRISPR's presence.

Because a microscope is required to see the glow from GFP, the researchers improved on their original method by replacing GFP with a similar reporter protein, called eYGFPuv, that is visible under black light, a type of ultraviolet light.

"Now we can see whether CRISPR is active in real time regardless of the size, shape and location of the organisms we're evaluating," Abraham said. "This flexibility speeds the bioengineering process and extends the biosensors' use in laboratory and field applications."

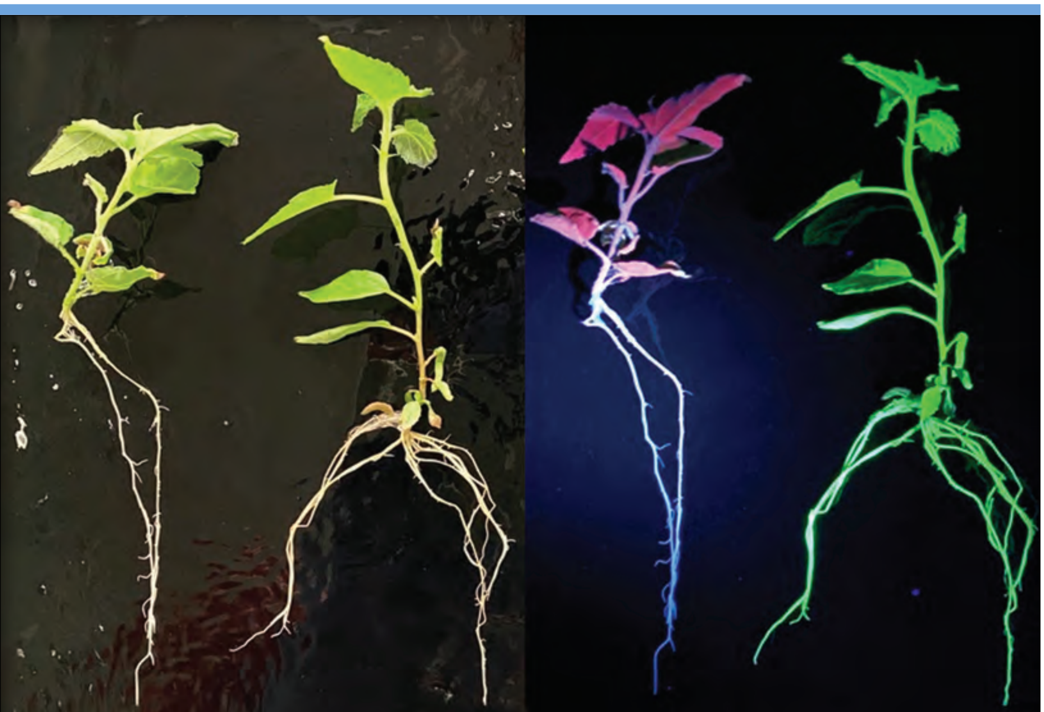
Because CRISPR must be tailored to each organism for effective use, knowing whether the CRISPR technology is working in a particular plant or microbe can accelerate progress toward goals such as developing drought-resistant bioenergy crops and engineering bacteria to effi-



ORNL's biosensor system provides an efficient self-detect solution that takes advantage of the way CRISPR (white) works to trigger the technology to reveal itself. The green fluorescent proteins signal CRISPR's presence. Image credit: Michelle Lehman, ORNL

ciently convert plants into sustainable aviation fuels.

The biosensors also provide an effective method to determine whether CRISPR is still active after the desired modifications have taken effect. ORNL plant synthetic biologist Xiaohan Yang compares CRISPR's genome editing activity to a beneficial surgery but cautions that "you don't want the surgeon to leave the scissors behind," as continued CRISPR activity could have unintended effects.



Yang envisions biosensor applications that could test the progeny of modified plants, for instance, to verify that the gene editing machinery did not transfer to them. With this technology, it is possible to survey an entire field of crops.

The team created specific biosensors to detect various CRISPR tools, including Cas9 nuclease, prime editor, base editor and CRISPRa. Abraham sees the potential to combine the biosensors into a version that would flag multiple gene editing technologies at once.

"We'll continue to optimize these biosensors to improve the security of next-generation biotechnologies," Abraham said.

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

ORNL's biosensor system reveals CRISPR activity in poplar plants, which glow bright green under ultraviolet light, compared to normal plants, which appear red. Image credit: Guoliang Yuan, ORNL

Predicting the planet's future

ORNL is deeply involved in the race to mitigate climate change. With a staff of world-class experts in fields ranging from ecology to chemistry to computer science and the nation's most powerful supercomputer, the lab helps us understand the problems that lie ahead and evaluate potential solutions.

Collecting critical data

ORNL both leads and collaborates in large-scale boots-on-the-ground experiments worldwide; it also houses troves of data collected by DOE, NASA and other agencies. This data feeds the DOE Energy Exascale Earth System Model, or E3SM.

- Atmospheric Radiation Measurement Data Center collects and shares millions of measurements from around the world of clouds, air particles, barometric pressure, etc.
- SPRUCE experiment, led by ORNL, exposes portions of a peat bog to a range of possible climate futures by raising temperatures and CO_2 levels in enclosed plots. Peat bogs hold at least one-third of the world's soil carbon.
- NGEE Arctic project, led by ORNL, improves understanding of the implications of a rapidly thawing Arctic tundra through measurements and modeling. (NGEE stands for "Next-Generation Ecosystem Experiments.")
- NGEE Tropics project, in which ORNL is a key partner, analyzes tropical forest responses to a changing climate.
- Earth System Grid Federation, led by ORNL, archives and distributes model output from international sources to inform global and regional climate change assessments.
- ORNL Distributed Active Archive Center houses and distributes data from NASA terrestrial ecology missions.

Designing a powerful model

DOE's E3SM model translates natural processes into equations that simulate complex interactions among:

- Land (e.g., how permafrost thaw in the Arctic triggers microbes to release ancient carbon from previously frozen soil)
- Ocean (e.g., how currents and circulation patterns influence the amount of plankton and seaweed)
- Atmosphere (e.g., how particles in the air absorb or reflect the sun's heat)
- Ice (e.g., how ice melt drives rising sea levels)
- Society (e.g., how future decisions about climate change mitigation could influence natural ecosystems)

Leveraging the world's most powerful supercomputers

- E3SM uses supercomputers to run simulations of Earth's complex systems with the detail necessary to inform decision-makers.
- E3SM currently uses ORNL's Summit supercomputer and will soon run on ORNL's new Frontier supercomputer, which is the world's first exascale system, capable of more than a quintillion calculations per second.
- Researchers test and verify model projections using data from the past several centuries before predicting the future.

Informing decision-makers

Climate models inform adaptation and mitigation strategies at the local, national and global level. ORNL climate scientists are:

- Contributing to landmark government reports such as the Intergovernmental Panel on Climate Change and the Fifth National Climate Assessment
- Assessing the climate resiliency of infrastructure and cities
- Modeling future climate impacts at neighborhood scales
- Projecting the impacts of clean energy technologies
- Examining how climate changes will shape future:
  - electricity demand
  - heat waves
  - drought
  - extreme weather
  - coastlines
- Simulating the effects on national security, including population movements and supply chain effects

Image credit: Brett Hopwood, ORNL

Mothers (and fathers) of invention:

Getting ORNL tech into the world

Do you ever wonder how discoveries made at America's national laboratories help American business? We asked ORNL Director of Technology Transfer Mike Paulus to shed a little light on the subject and to share the lab's top 10 technology transfer success stories.

Mike Ramsey (pictured) and Stephen Jacobson pioneered the development of the lab on a chip for rapid, inexpensive biological and chemical analyses. Image credit: ORNL

by Jim Pearce
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The best partner possible

ORNL scientists clearly invent technologies and processes, and the laboratory wants to make them available to U.S. companies with the goal of improving the national economy.

"A lot of our research output is put into the public domain in scientific publications," ORNL Director of Technology Transfer Mike Paulus said, "but there are times when companies have to make large investments to turn our scientific results into products or services, so they need some exclusivity in order to get a return on their investment."

To make these matches, Paulus' team has to align the needs of both researchers and businesses.

"Our first job is to help researchers identify inventions that could have commercial potential and work with them to patent these inventions," Paulus said. "Our second job is to engage with businesses, connect them with the researchers, provide them with the intellectual property they need to succeed, and then, often, to continue to take advantage of the laboratory's capabilities."

Tech transfer successes

When these pairings succeed, ORNL technologies are licensed, refined and brought to market by companies in the private sector. Royalty fees are managed by ORNL contractor UT-Battelle with oversight from DOE.

What follows are the laboratory's top 10 technology transfer successes based on licensing revenue.

1 Lab on a chip — In 1987, ORNL chemists Mike Ramsey and Stephen Jacobson devised a way to speed up chemical separations processes by passing small samples through what amounted to a tiny chemistry lab etched into a glass microscope slide.

"They came up with a really innovative way to do high-throughput, flexible chemistry," Paulus said. "Their invention got out in front of a market that was growing rapidly."

Ramsey and Jacobson patented the device in 1995, and Ramsey co-founded a company, Caliper Technology Corporation, to further develop the technology. The "lab on a chip" concept has evolved to encompass genetics research, pharmaceutical development and other biochemical separations processes.

2 Wireless temperature sensors — In 1994, while ORNL scientists Bob Lauf and Don Bible were attending a meeting at Sematech, they learned of an industry problem: Wires from the sensors used to ensure uniform heating of semiconductor chips were getting in the way and affecting the reliability of measurements.

"As I understand it," Paulus said, "Lauf and Bible went to a bar, pulled out a napkin, sketched an idea, came home, and — with the help of ORNL engineer Carl Sohns — built a prototype and filed a patent. Then they went back to the [Sematech] representative and said, 'We have a solution: a wireless temperature sensor.'"

ORNL licensed the patent to SensArray in 2001, and in 2005 the SensArray Integrated Wafer won Semiconductor International and R&D 100 awards.

3 Silicon carbide whisker-reinforced ceramic composites for cutting tools — In the early 1980s, ORNL's George Wei, Terry Tiegs and Paul Becher created a ceramic composite reinforced with silicon carbide whiskers — like rebar in concrete — making it ideal for cutting tools and other wear-resistant applications. The technology was licensed in 1986 to Advanced Composite Materials Corp. and was later distributed by Greenleaf Tooling Solutions.

Carl Sohns, Bob Lauf and Don Bible (left to right) are shown in 2005 with their wireless temperature sensor. The sensor helps to ensure uniform heating of semiconductor chips.
Image credit: Curtis Boles, ORNL

"The material was really successful in tooling applications," Paulus said. "Those guys are still selling products based on this material, and the technology is still making a difference long after the patents expired."

4 Handheld mass spectrometry system — Ramsey, the same researcher who co-developed "lab on a chip," worked with ORNL's Bill Whitten to develop a handheld mass spectrometer, which is used to identify the composition of samples in fields like materials science, forensics, pharmaceuticals, biology and chemistry. The technology was licensed to 908 Devices in 2012. ORNL received equity in the company as a part of the licensing fee, so when its $150 million initial public offering closed in December 2020, ORNL was able to sell its stock.

"That was the first stock sale that we've had since I've been here," Paulus said. "That was an exciting day for the lab."

5 RABiTS (Rolling-Assisted Biaxial Textured Substrate) — In 1996, ORNL scientists Amit Goyal and Parans Paranthaman led the development of new methods and materials for producing high-temperature superconducting materials. The work was supported by a cooperative research and development agreement, or CRADA, with American Semiconductor, and one of the technologies was licensed to the company in 2000. A second technology was licensed to SuperPower Inc. in 2007.

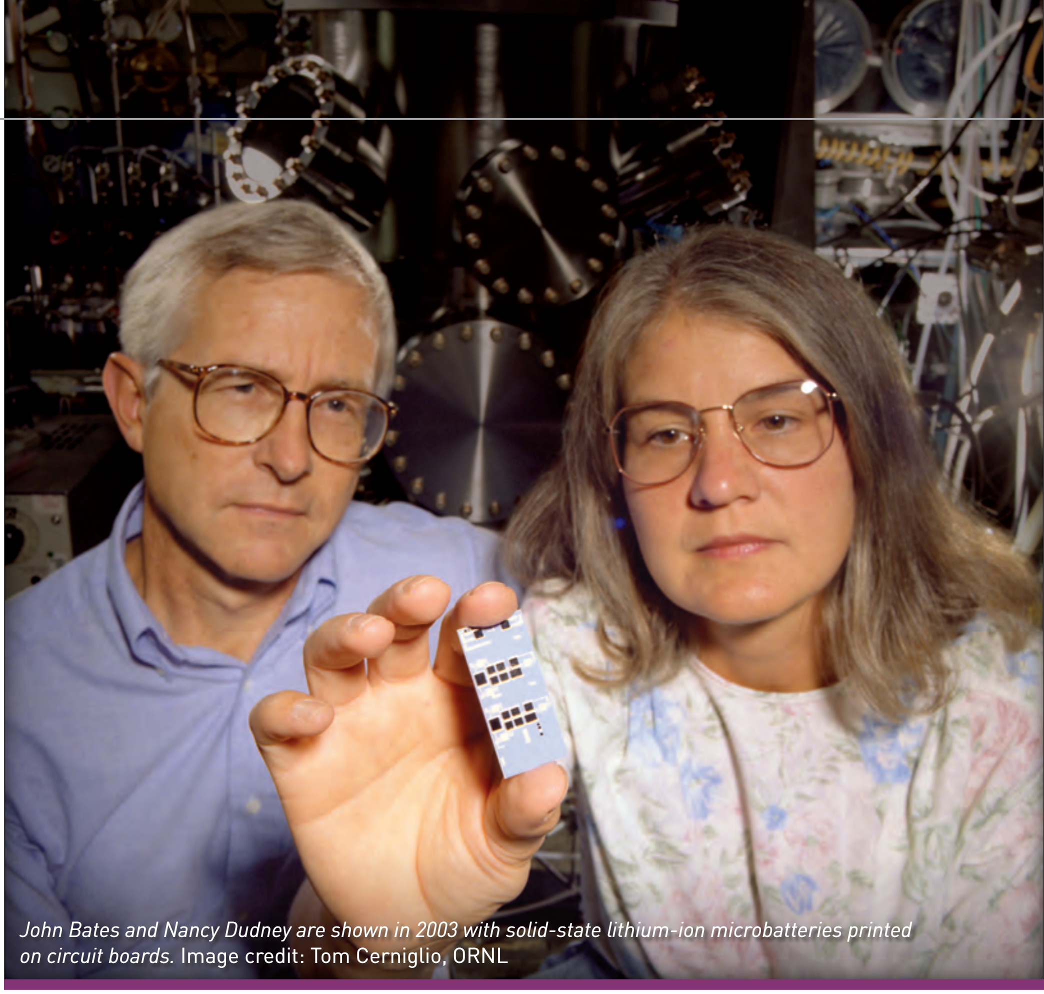
"This is an example of a sustained, focused program funded by DOE to advance a technology that resulted in a huge patent portfolio and companies," Paulus said.

6 Thin-film, solid-state battery technology — "Nancy Dudney, John Bates and Bernd Neudecker developed a solid-state electrolyte technology in the 1990s that enabled very small batteries to be printed on circuit boards using semiconductor technology," Paulus said.

See MOTHERS (AND FATHERS), page 40

MOTHERS (AND FATHERS), page 39

The technology was developed through a handful of CRADAs and was eventually licensed to several companies, each of which marketed solid-state lithium-ion microbatteries. These thin-film batteries are longer lasting, more robust and safer than the current generation of liquid electrolyte–based lithium-ion batteries.



John Bates and Nancy Dudney are shown in 2003 with solid-state lithium-ion microbatteries printed on circuit boards. Image credit: Tom Cerniglio, ORNL

7 **Bio-succinic acid process** — The aim of this project was to find a way to produce succinic acid — a building block for numerous chemical products — that did not rely on petroleum-based chemicals. ORNL scientists Nhuan Nghiem and Brian Davison collaborated with colleagues at Argonne National Laboratory and the National Renewable Energy Laboratory to do just that, devising a microbial process for creating succinic from biomass. A patent for the technology was filed in 1997, and the technology was later licensed by Applied CarboChemicals, which, after a merger, became JV BioAmber. The company built a demonstration plant in France in 2010 and operated it for several years.

Parans Paranthaman's RABITS technology has been used to make an iron-based superconducting wire capable of carrying very high electrical currents under exceptionally high magnetic fields. Paranthaman is shown here in 1996. Image credit: Tom Cerniglio, ORNL

8 **LandScan** — The LandScan database combines a range of data, including census information and satellite imagery, to produce very-high-resolution, graphical representations of global population distribution. It was developed in 1998 by ORNL scientists Budhu Bhaduri, Phillip Coleman, Edward Bright, Amy Rose and Marie Urban.

Some of LandScan's biggest impacts have been seen during times of natural disaster, when relief agencies ask researchers to use the database to predict where people impacted by events such as earthquakes, tornadoes and tsunamis will go when they evacuate. This capability enables agencies to deliver relief supplies and other resources to the right places.

LandScan was licensed to East View Geospatial from 2012 to 2021. It has been distributed through an open-source license for academic use since 2021.

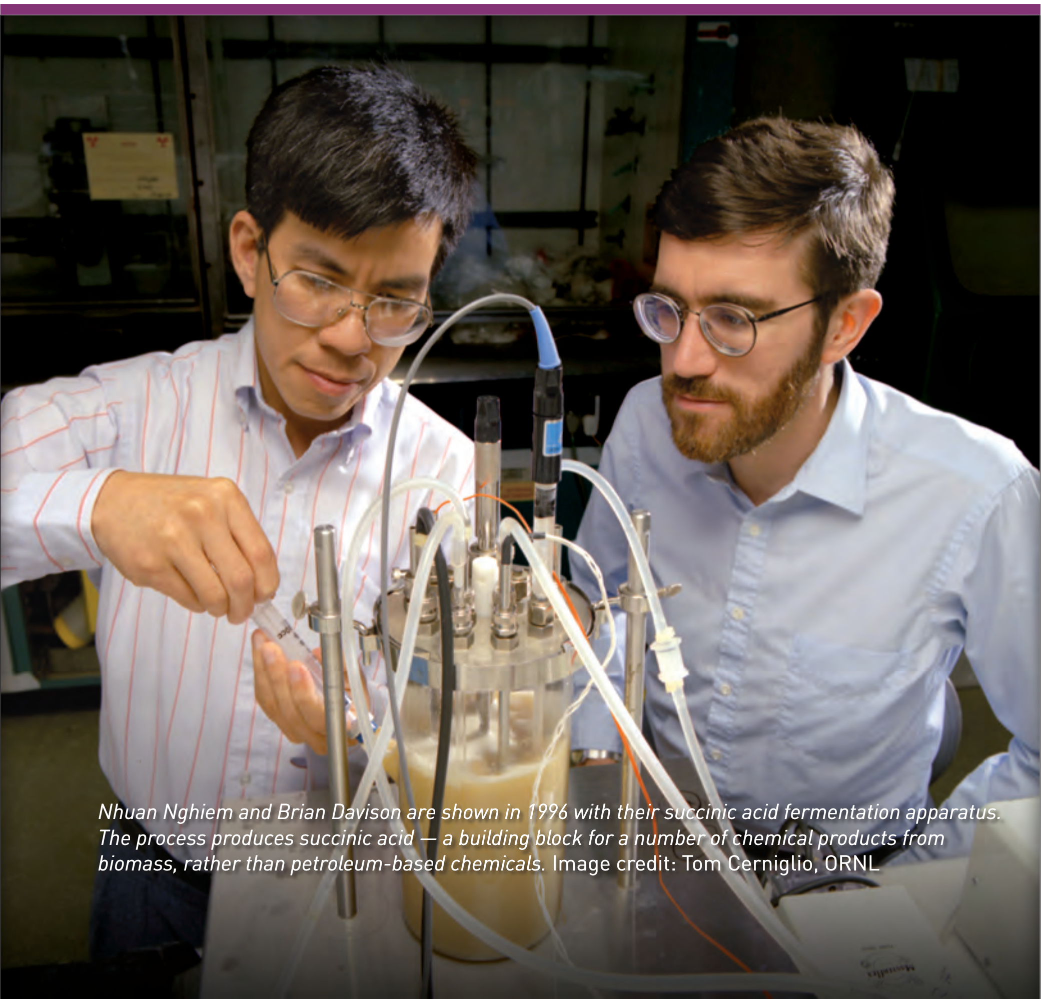
9 **Content-based image retrieval system for improving semiconductor yield** — "I see ORNL's Automated Image Retrieval Technology — AIR — as a precursor to artificial intelligence–based image analysis," Paulus said. "It was

developed by ORNL scientists Ken Tobin, Regina Ferrell, Tom Karnowski, Shaun Gleason and Hamed Sari-Sarraf."

The researchers compiled a database of known defects in semiconductor processing, then built a tool, AIR, to enable users to quickly compare images of problematic semiconductor wafers with those in the database. Based on that comparison, they can determine what went wrong in the manufacturing process. AIR was licensed in 2004 to August Technology Corporation and was marketed under the trade name TrueADC.

10 **Open port sampling interfaces for mass spectrometry** — ORNL chemists Gary van Berkel and Vilmos Kertesz have specialized in developing innovative interfaces between mass spectrometry systems and samples. In this case, their innovation enables even novice users to load solid or liquid samples into a mass spectrometer and achieve reliable results.

Gary Van Berkel (left) and Vilmos Kertesz are shown in 2017 with their open port sampling interface. The technology enables easy, sensitive and rapid chemical analysis by mass spectrometry. Image credit: Jason Richards, ORNL



Nhuan Nghiem and Brian Davison are shown in 1996 with their succinic acid fermentation apparatus. The process produces succinic acid — a building block for a number of chemical products from biomass, rather than petroleum-based chemicals. Image credit: Tom Cerniglio, ORNL

"This is an overnight success that took more than 20 years," Paulus observed wryly. "ORNL has partnered with SCIEX since 1996. In that time, we've had multiple cooperative R&D agreements. In 2022, SCIEX launched a new flagship mass spectrometry system, and our technology is an integral part of that system."

Always opportunities to do things better

Each of these technology transfers was enabled by the Bayh-Dole Act of 1980, the law that allows universities, national laboratories and small businesses to patent and profit from discoveries made through federally funded research.

"It has been said that the Bayh-Dole Act is possibly the most inspired piece of legislation to be enacted in the U.S. over the past half century," Paulus said.

"The incentive it provides has made a big difference in moving R&D from federal laboratories to business and industry in the U.S. Empowering institutions that invent to connect with companies that produce ensures that there's a direct path into the marketplace."

Decarbonization:

Q&A with David Sholl

by Stephanie Seay
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David Sholl joined ORNL as director of the Transformational Decarbonization Initiative in July 2021. He is working to elevate the lab's decarbonization science and technology, including carbon capture, conversion and storage.

Sholl holds a joint appointment with the School of Chemical and Biomolecular Engineering at Georgia Tech. He is a fellow of the American Association for the Advancement of Science and the American Institute of Chemical Engineers. Sholl earned his Ph.D. and master's degree in applied mathematics from the University of Colorado, and a bachelor's in theoretical physics from The Australian National University.

What are the goals of the TDI?

The Transformational Decarbonization Initiative at ORNL is focusing its efforts in three areas. One of these is focused solutions for sectors of the economy that will be difficult to decarbonize. A good example is off-road and heavy-duty transportation such as aviation, large ships, farm equipment and long-haul trucks. These applications are hard to electrify due to space and weight considerations. Even with increased use of bio-based fuels, this sector will have significant CO_2 emissions for a very long time. We are working on carbon-negative technologies such as capturing CO_2 directly from air that will be needed to get to a truly net-zero emissions economy.

Second, we are funding projects at the lab to convert CO_2 into useful products, anticipating very large quantities of captured CO_2 in the future. If we are hugely successful in CO_2 mitigation, we will be generating perhaps a billion tons a year of it in the United States, about the same size as the U.S. petrochemicals industry today. We know scientifically how to do all of these things. The challenge is to develop solutions that are affordable and work at very large scales.

A third area we're looking at is the global impact of capturing CO_2. We want to better understand the potential impacts on natural carbon sinks such as oceans and soils and the general effect on plants in our biosphere as we achieve CO_2 capture. We will be using very large, very sophisticated computer models to

"Anything that will be relevant to climate change mitigation must be implemented at a gigantic scale. To me, the implication of this is that no individual person can solve the problem. You need expertise from many, many fields.

— Transformational Decarbonization Initiative Director **David Sholl**

understand those feedbacks and to better predict impact on the future climate.

How does TDI fit into DOE's Energy Earthshots initiative?

DOE's Energy Earthshots are an all-hands approach for science and technology to meet the nation's climate and economic competitiveness goals. We take a similar approach here at ORNL. The breadth of our interdisciplinary expertise and capabilities means we can tackle the full range of technologies needed to address the climate challenge.

TDI is strongly aligned with DOE's Carbon Negative Earthshot. For example, we're not just looking at directly capturing CO_2; we're also looking at understanding carbon stored in soil. How do you even accurately detect and measure soil carbon? It varies from location to location. How long will that carbon stay in the soil given the very complicated interactions between the soil microbiome and the plants growing in it? Then there are things we can do in terms of trying to optimize our bioenergy crops. To me, this is a great example of how the interdisciplinary environment at Oak Ridge can help people develop big ideas and create the teams to make them a reality.

The climate challenge is enormous. Can we make a difference?

I believe so, yes. Anything that will be relevant to climate change mitigation must be implemented at a gigantic scale. To me, the implication of this is that no individual person can solve the problem. You need expertise from many, many fields. You need scientific expertise and engineering expertise and people who can think about life cycle analysis. You need people who can think about the economics and the equity issues associated with these very large-scale technologies. And you need to be able to connect with outside partners and industry. All this is something that we are very well suited to at the lab, and where we have a proven track record.

The challenge is so large that there will need to be many solutions. A colleague described it well recently when they said there is no silver bullet, but we can aim for silver buckshot.

Quick detection of uranium isotopes

helps safeguard nuclear materials

by Dawn Levy
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Analytical chemists from ORNL's Chemical and Isotopic Mass Spectrometry Group have developed a rapid way to measure isotopic ratios of uranium and plutonium collected on environmental swipes, which could help International Atomic Energy Agency analysts detect the presence of undeclared nuclear activities or material.

"This method builds on a commercial microextraction probe to directly sample solids and subsequently extract the analytes from a surface and into a flowing solution," said Benjamin Manard. He led a proof-of-concept study demonstrating that this sampling mechanism was effective at extracting actinide material (e.g., uranium and plutonium) from environmental swipes.

This innovation could help IAEA's Network of Analytical Laboratories, or NWAL, which includes ORNL, analyze samples collected from facilities worldwide.

"The microextraction method, if it achieves suitable precision and accuracy, could enable higher sample throughput and faster turnaround time," said DOE NWAL coordinator and ORNL study partner Brian Ticknor.

A pen-sized microextraction probe uses a "wet vacuum" to mobilize material from a swipe surface. Manard's team couples the probe to an instrument that subjects the extracted material to a plasma — an ionized gas hotter than the surface of the sun — and measures the mass-to-charge ratios of the ions generated from the sample.

"It truly is an integrated system," Manard said. "With just a click of a button, you're going from a solid sample on a swipe to an isotopic measurement."

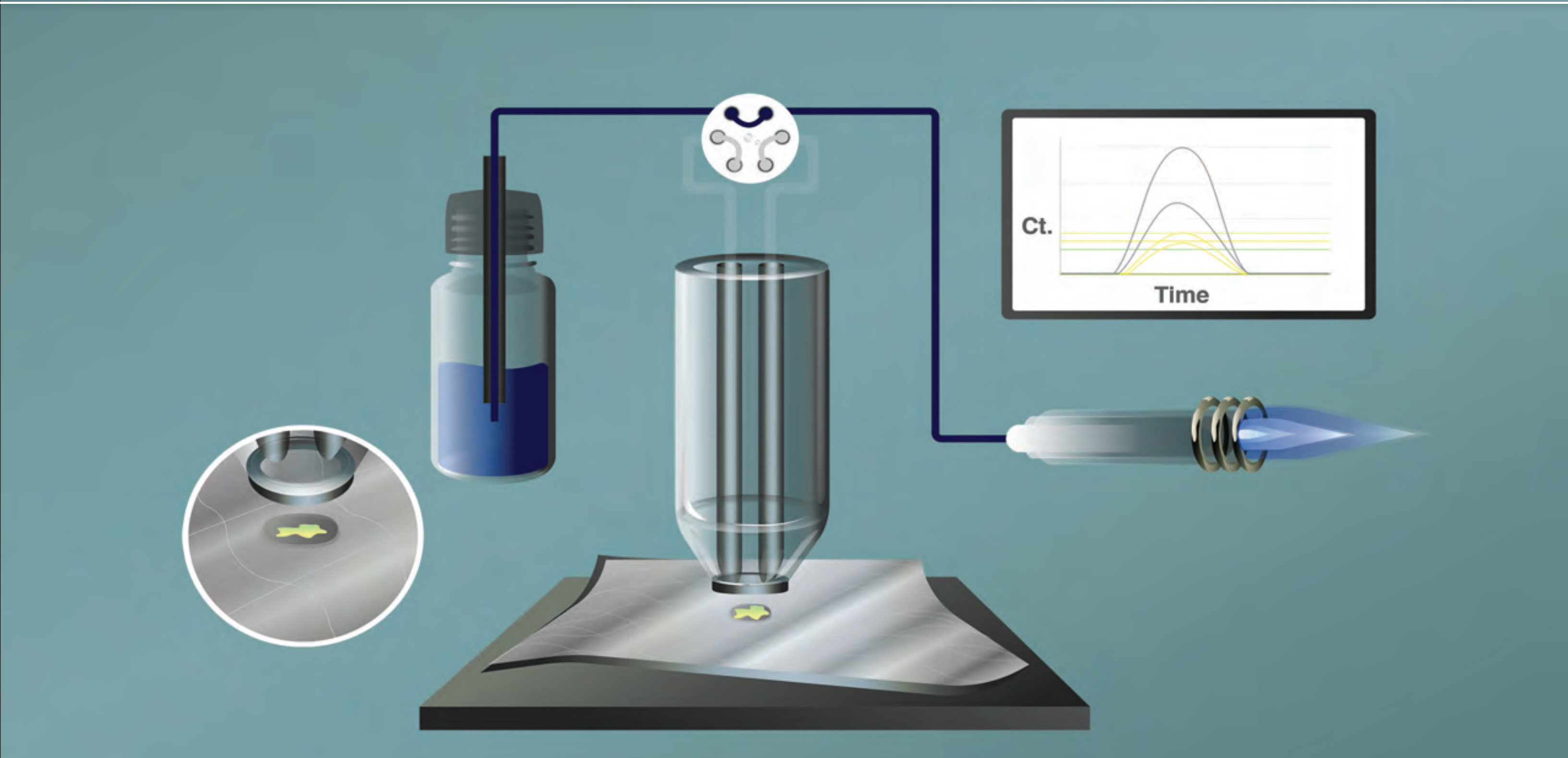
With this novel approach to assaying solids, Kayron Rogers made a series of swipe samples containing varying amounts of reference standards. The team was able to detect as little as 50 picograms of uranium — 80 million times lighter than a grain of sand. Moreover, the researchers made precise and accurate measurements of the ratios of major and minor isotopes of elements in nuclear reference materials. In a subsequent study, they applied the technique to the analysis of plutonium.

"The benefits of this methodology could extend beyond nuclear material analysis to many applications requiring direct elemental analysis," Manard said.

Traditionally, analysts turn inspection samples to ash in a furnace before acid digestion and lengthy chemical separations. The process, from creating the ash to analysis, could typically take up to 30 days. "The goal of this project was to cut down on those steps in the beginning — ashing and dissolution," Manard said. "If we could sample the swipe directly, we don't have to go through the process of trying to turn a swipe into a liquid."

The researchers work in ORNL's Ultra-Trace Forensic Science Center, a service center and research facility providing expertise and state-of-the-art inorganic mass spectrometry instrumentation.

A team led by ORNL's Benjamin Manard developed a rapid way to measure isotopic ratios, which could speed analyses supporting inspections of nuclear facilities. Image credit: Carlos Jones, ORNL



ORNL's rapid isotope measurement system extracts a solid from a swipe, ionizes it with a plasma torch and measures the mass-to-charge ratio of the sample's ions with a mass spectrometer. Image credit: Jaimee Janiga and Michelle Lehman, ORNL

"This project brings together ideas and technologies developed at ORNL that could provide the next revolutionary change to environmental sampling methodology," said Cole Hexel, who worked on the study and leads the group.

The researchers are excited about experiments to be conducted over the next two years that will examine the versatility of the methodology.

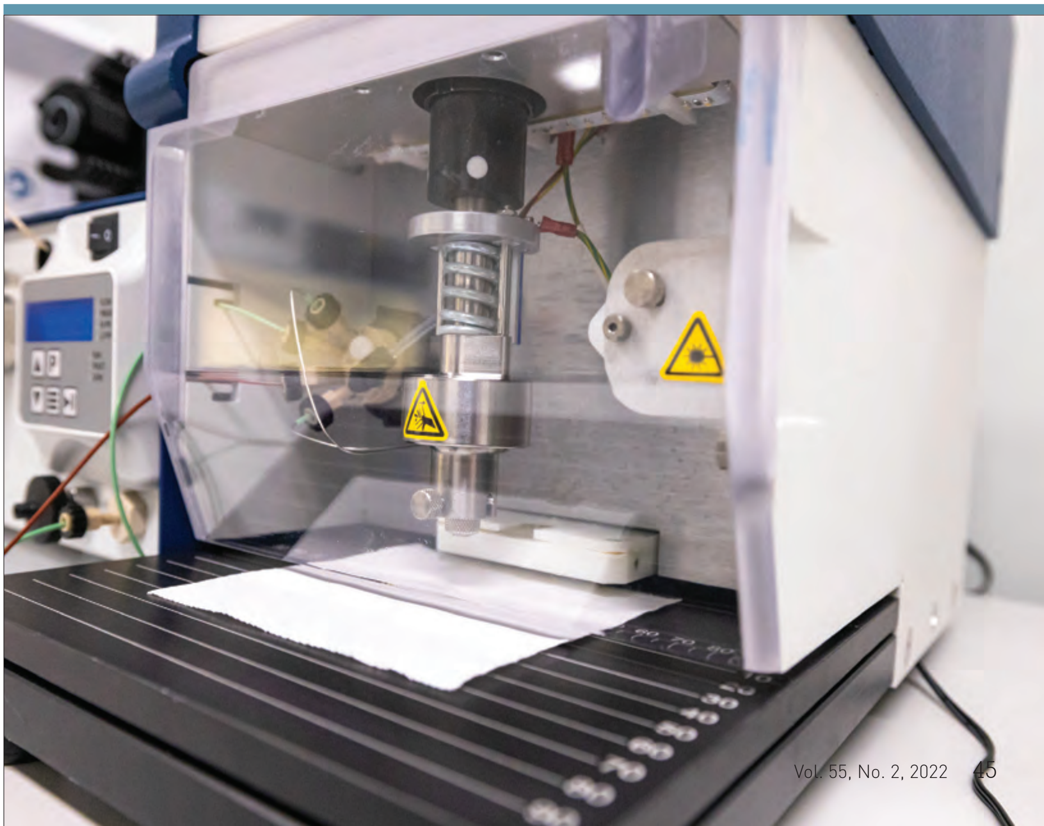
An innovative approach led by Shalina Metzger involves putting a chromatography column between the microextraction probe and the mass spectrometer and having actinide-containing solutions flow through connective tubing. Whereas the column would allow uranium to flow through, it would retain plutonium for measurement and later removal with a solvent. The approach would improve elemental sensitivity and identification.

During their studies, the researchers found that nitric acid degraded the microextraction probe head. Future experiments will seek to optimize solvent conditions for extracting actinides in various chemical forms.

"We're also using ORNL's unique 3D-printing facilities to fabricate components with polymers that are more resistant to the extraction solvent," Manard said.

Ultimately, the ORNL researchers hope to develop the capability to differentiate individual analytes collected on a swipe to provide an overall snapshot of an inspected facility's activities.

For more information: https://go.usa.gov/xz7ks



ORNL analytical chemists coupled a microextraction probe to a mass spectrometer for measurement of uranium isotope ratios from environmental swipes. Image credit: Carlos Jones, ORNL

Upcycled:

From common plastic to tough, recyclable adhesive

by Ashley Huff
huffac@ornl.gov

Commodity plastics used globally for toys, household goods and food containers generate millions of tons of plastic waste each year, most of which is not recycled and accumulates in the environment. Tackling this crisis will require fundamental breakthroughs that reduce waste, drive reuse and add value to recycled materials.

Polymer chemists at ORNL are exploring "upcycling" strategies that incorporate new functionality into common plastics, such as adding industrial strength to an everyday material — a step that could give disposable plastics new purpose with properties tailored for specialized tasks.

Researchers Tomonori Saito and Md Anisur Rahman used polymer chemistry to transform a common household plastic into a reusable adhesive with a rare combination of strength and ductility, making it one of the toughest materials ever reported.

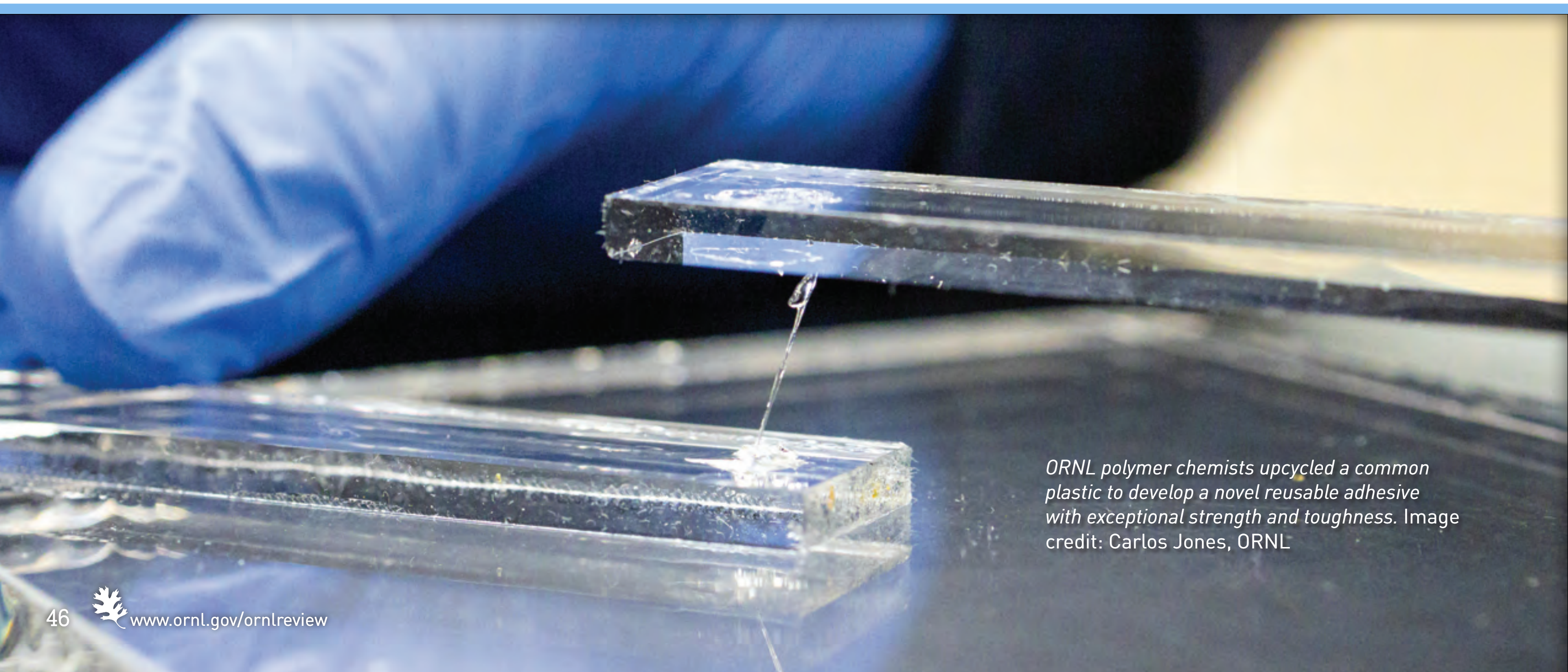
The team aimed to upcycle polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene, or SEBS — a rubbery plastic used in products ranging from toys to electronics to footware that is easy to process but not engineered for tough adhesion. Their work fundamentally advances pathways to design a new class of tough adhesives with desirable features merged into a single material. The technology adapts to bear heavy loads, tolerate extreme stress and heat, and reversibly bond to various surfaces including glass, aluminum and steel.

"Strong, tough adhesives are difficult to design because they need to incorporate hard and soft features that are not typically compatible," Saito said.

Structural adhesives such as epoxy are largely designed for load-bearing strength but lack toughness, a property that helps materials dissipate stress when pulled or stretched to prevent sudden failure.

"The challenge has been to add the toughness you get in flexible materials without sacrificing strength. Our approach uses dynamic chemical bonds to develop a novel adhesive with remarkable properties not seen in current materials," Saito said.

The team modified SEBS' chemical structure with dynamic crosslinking to



ORNL polymer chemists upcycled a common plastic to develop a novel reusable adhesive with exceptional strength and toughness. Image credit: Carlos Jones, ORNL

ORNL scientists Md Anisur Rahman (left) and Tomonori Saito demonstrate the load-bearing strength of a novel tough adhesive developed for challenging applications. A drop of adhesive the size of 1 square centimeter can hold approximately 300 pounds. Image credit: Carlos Jones, ORNL

make it more robust. Crosslinking is a known strategy for designing materials with more stable properties. The approach can create a bridge between structures that are not normally compatible. The team created a novel composite material by using boronic esters to couple SEBS with silica nanoparticles, a filler material used to strengthen polymers.

Conventional crosslinking typically results in permanent bonds that prevent adhesives from being removed or reprocessed. The study found that boronic esters enable "dynamic" or reversible crosslinking and are key to the new material's strong adhesion and recyclability. These unique chemical compounds can create stable bonds that can make and break repeatedly — an unusual feature that makes them attractive for sustainable materials design.

Results showed crosslinked bonds shift within the material to enable specific properties and adhere to surfaces so strongly that a thin square centimeter can hold roughly 300 pounds. Shear tests that measure toughness by trying to detach materials with force widely exceeded all commercial adhesives tested in the study. The material was so tough in adhering to glass, in fact, that glass fractured before the sample debonded. The approach also enhanced thermal stability to 400 degrees Fahrenheit, making the adhesive attractive for both ambient and high-temperature applications.

In addition to extraordinary adhesion, a surprising property of the tough material is that it can also be recycled. "It is rare for a high-performance adhesive to be removable, but ours is designed for reuse and recyclability," Rahman said. "It can be applied and detached with heat and pressure and reused several times."

The novel adhesive could advance challenging applications in the aerospace, automotive and construction industries, and its reusable design offers benefits to industry and the environment. Moreover, the fundamental science opens pathways for optimizing new tough adhesives for numerous bonding applications.

Tiny but mighty

precipitates toughen a structural alloy

by Dawn Levy
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Scientists at ORNL and the University of Tennessee, Knoxville, have found a way to increase both the strength and ductility of an alloy by introducing tiny bifunctional precipitates into its matrix and tuning their size and spacing. The precipitates are solids that separate from the metal mixture as the alloy cools.

Results of this work will open new avenues for advancing structural materials.

Ductility is a measure of a material's ability to undergo permanent deformation without breaking. It determines, among other things, how much a material can elongate before fracturing and whether that fracturing will be graceful or catastrophic. The higher the strength and ductility, the tougher the material.

"A holy grail of structural materials has long been, how do you simultaneously enhance strength and ductility?" said Easo George, principal investigator of the study and Governor's Chair for Advanced Alloy Theory and Development at ORNL and UT. "Defeating the strength–ductility trade-off will enable a new generation of lightweight, strong, damage-tolerant materials."

If structural materials could become stronger and more ductile, components of cars, planes, power plants, buildings and bridges could be built using less material. Lighter-weight vehicles would be more energy-efficient to make and operate, and tougher infrastructure would be more resilient.

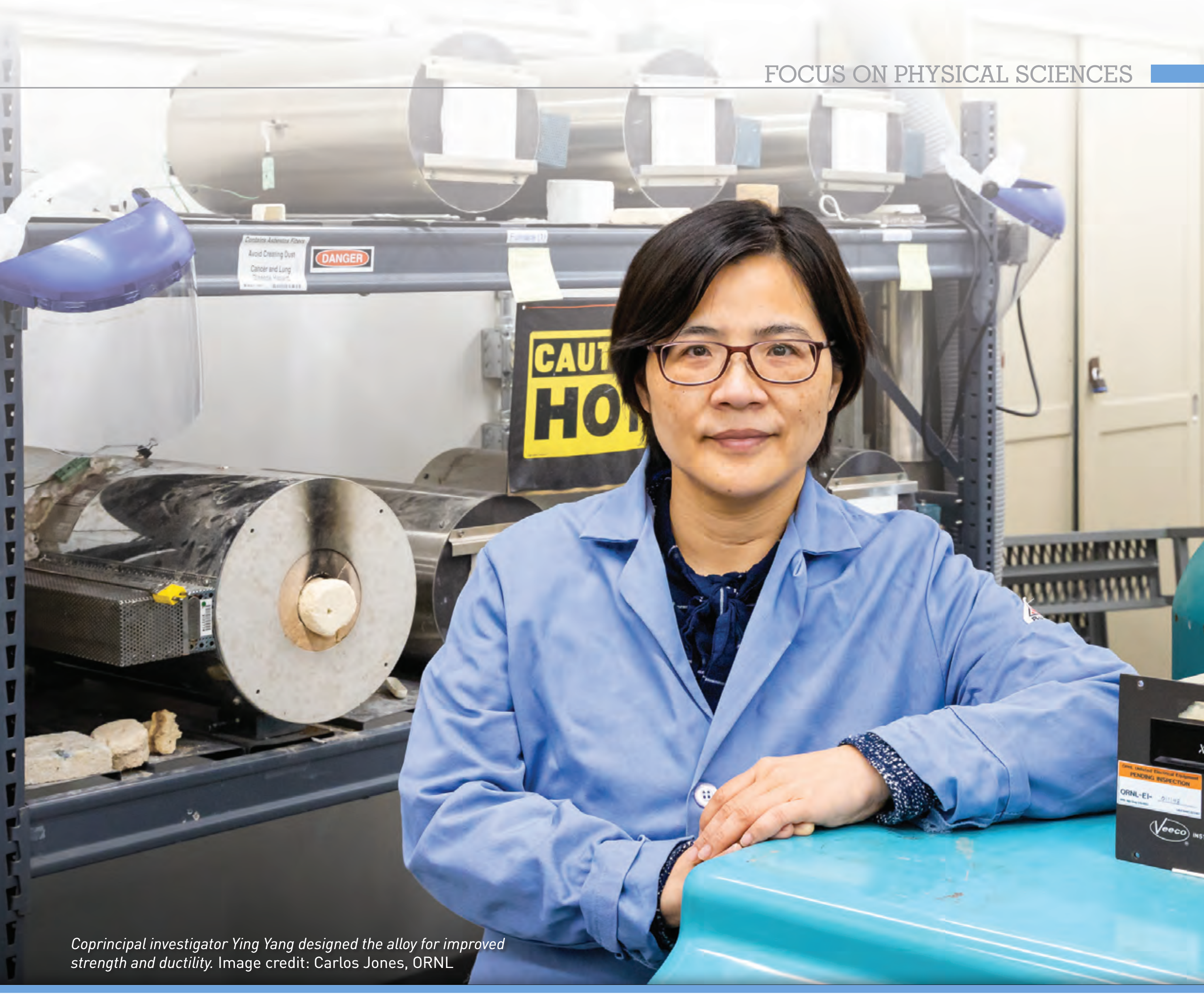
> *"A holy grail of structural materials has long been, how do you simultaneously enhance strength and ductility? Defeating the strength–ductility trade-off will enable a new generation of lightweight, strong, damage-tolerant materials.*
>
> — University of Tennessee and ORNL Governor's Chair for Advanced Alloy Theory and Development **Easo George**

Co-principal investigator Ying Yang of ORNL conceived and led the study. Guided by computational thermodynamics simulations, she designed and custom-made model alloys with the special ability to undergo a phase transformation driven by changes in either temperature or stress. The cubic cells making up the material's lattice change from a face-centered cubic, or FCC, crystal structure — in which atoms sit at the corners and the centers of each face — to a body-centered cubic, or BCC, crystal structure — in which atoms sit at the corners and the center of the cube.

"We put nanoprecipitates into a transformable matrix and carefully controlled their attributes, which in turn controlled when and how the matrix transformed," Yang said. "In this material, we intentionally induced the matrix to have the capability to undergo a phase transformation."

The alloy contains four major elements — iron, nickel, aluminum and titanium — that form the matrix and precipitates, and three minor elements — carbon, zirconium and boron — that limit the size of grains, or individual metallic crystals.

The researchers carefully kept the composition of the matrix and the total amount of nanoprecipitates the same in different samples. However, they varied precipitate sizes and spacings by adjusting the processing temperature and time.



Coprincipal investigator Ying Yang designed the alloy for improved strength and ductility. Image credit: Carlos Jones, ORNL

"The strength of a material usually depends on how close the precipitates are to each other," George said. "When you make them a few nanometers [billionths of a meter] in size, they can be very closely spaced. The more closely spaced they are, the stronger the material gets."

While nanoprecipitates in conventional alloys can make them super-strong, they also make the alloys very brittle. The team's alloy avoids this brittleness because the precipitates perform a second useful function: by spatially constraining the matrix, they prevent it from transforming during a thermal quench — a quick immersion in water that cools the alloy to room temperature.

Consequently, the matrix remains in a metastable FCC state. When the alloy is then stretched —"strained" as researchers call it — it progressively transforms from metastable FCC to stable BCC. This phase transformation during straining increases strength while maintaining adequate ductility.

In contrast, an alloy without precipitates transforms fully to stable FCC during the thermal quench, which precludes further transformation during straining. As a result, it is both weaker and less ductile than the alloy with precipitates. Together, the complementary mechanisms of conventional precipitation strengthening and deformation-induced transformation increased strength by 20 to 90 percent and elongation by 300 percent.

Next, the team will investigate additional factors and deformation mechanisms to identify combinations that could further improve mechanical properties.

It turns out, there is a lot of room for improvement.

"Today's structural materials realize but a small fraction — perhaps only 10 percent — of their theoretically capable strengths," George said. "Imagine the weight savings that would be possible in a car or an airplane — and the consequent energy savings — if this strength could be doubled or tripled while maintaining adequate ductility."

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

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.

Kevin De Angeli

Graduate student, Computational Sciences and Engineering Division
Ph.D. student, Data Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Buenos Aires, Argentina

What are you working on at ORNL?

My research focuses on developing and improving machine learning models to classify cancer pathology reports. Information extraction from clinical reports is an expensive, time-consuming task that is performed by experts. By building robust deep learning models, we hope to expand our understanding of cancer trends across the U.S.

What would you like to do in your career?

I want to continue developing and applying data science tools to help communities and create more opportunities for future generations. Throughout my years in academia, I have learned the importance of good mentorship, so I would also like to mentor the future generation of scientists.

Why did you choose a career in science?

I have always enjoyed mathematics and computer science. By pursuing data science, I am able to work at the intersection of both fields while solving real-world problems that can potentially have an impact in society.

Joni Hall

Graduate student, Electrification and Energy Infrastructure Division
Ph.D. Student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Kingston, Jamaica

What are you working on at ORNL?

My work focuses on strategies that enable residential electricity customers to automate decision-making related to devices ranging from HVAC systems to electric vehicles, in a manner that benefits them and the grid. Homes are no longer just consumers of electricity, but also resources with adjustable demand and supply capabilities.

What would you like to do in your career?

Our ability to harness energy has been transformative, but it has also created challenges. I would like to contribute to finding solutions which overcome the challenges created by our current energy system, helping to move it toward being sustainable while helping to equip the next generation of problem solvers.

Why did you choose a career in science?

There are many things I find interesting, and what they have in common is they provide opportunities to find solutions. Science provides a framework and tools for exploration and problem solving. Solving real-world problems brings me joy, so I found science a natural fit.

Vasudevan Iyer

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Mechanical Engineering, Purdue University
Hometown: Coimbatore, India

What are you working on at ORNL?

I'm studying nanomaterials such as 2D semiconductors, nanoantennas, perovskites and plasmonic structures using laser spectroscopy and electron microscopy. My interest lies in characterization of these materials at high spatial and temporal resolution to uncover novel physics. These materials have applications in the energy, communications and computing sectors.

What would you like to do in your career?

I want to continue my research in the field of nanotechnology either as a scientist or a faculty member. I'm excited to utilize my skills for solving the energy and climate challenges our generation faces.

Why did you choose a career in science?

I am always fascinated to experience technology, be it the first time I sat on a plane or when we got our first computer at home. I used to ask my mother what I could invent that would make her proud. I naturally gravitated towards science in high school and was fortunate to get into a good college.

Yessica Alejandra Nelson

Graduate student, Neutron Scattering Division
Ph.D. Student, Inorganic Chemistry, UCLA
Hometown: Jalisco, Mexico

What are you working on at ORNL?

We design boron clusters at the atomic level, subject them to high pressures and use neutrons and X-rays to elucidate phase changes induced by the applied pressures. We hope to accelerate the design of solid-state inorganic electrolytes with superior ionic conductivity at room temperature for a new generation of all-solid-state batteries.

What would you like to do in your career?

As a scientist, I want to advance chemistry through an interdisciplinary and multicultural approach to solving critical energy and environmental problems while making knowledge accessible to all.

Why did you choose a career in science?

I witnessed how a lack of education and resources led to inadequate farming and sanitation practices affecting my hometown's environmental sustainability. I knew the only way to impart change was through science and education. I feel fortunate to spend my time immersed in problem solving and helping the next generation of scientists.

Darren Driscoll

Postdoc, Chemical Sciences Division
Ph.D., Chemistry, Virginia Tech
Hometown: Haymarket, Virginia

What are you working on at ORNL?

My current research focuses on understanding local and mesoscale structure during the extraction of rare earth elements. I utilize a combination of synchrotron-based X-ray and neutron techniques to describe rare earth element local coordination and aggregation within extraction mediums in an effort to tailor novel material development for increased separation efficiency.

What would you like to do in your career?

I want to be a world expert in structural chemistry combining high-energy X-ray and neutron techniques to drive the next generation of energy science discoveries. I aspire to join other scientific experts in collaboration to solve complex scientific challenges impacting our modern society.

Why did you choose a career in science?

I like to think the career chooses the person. I enjoy the daily challenges and the overall successes that define me as a researcher.

Omy Tonia Ogbughalu

Postdoc, Biosciences Division
Ph.D., Systems Genetics and Biogeochemistry, University of South Australia
Hometown: Brisbane, Australia; Enugu, Nigeria

What are you working on at ORNL?

My research at ORNL is in systems genetics. Using a suite of molecular and computational tools, I characterize shifts in microbial — self-replicating plasmids, viruses, bacteria, fungi and algae — community structure, which may impact terrestrial and aquatic ecosystem function, to establish how urbanization alters the biogeochemical processes controlled by varied microbial interactions.

What would you like to do in your career?

I would like to develop novel biotechnological tools to predict biogeochemical function and to identify when microbes such as viruses intercept, infect or alter the metabolic activities of other microbial groups. These tools would be able to identify the networking strategies activated by different microbial groups in response to physical, mechanical or chemical perturbations.

Why did you choose a career in science?

I grew up being fascinated by ubiquitous, yet invisible, microbes. Microorganisms are the center of our existence and of medical, agricultural and environmental science. I believe that microbes hold the blueprint to our survival. They can make or mar us. So, for a sustainable environment, I choose to work with them.

Nurse Doris Scott bridged lab's early race–health disparity

by Bill Cabage
cabagewh@ornl.gov

When in 1948 Doris Belle Scott, just graduated from Meharry Medical College School of Nursing, sat for her interview for a position at ORNL, the medical director, J.S. Felton, explained the laboratory's philosophy of industrial health: "That the maintenance of a worker's health is as important after the whistle blows as before, and that every employee, irrespective of his or her position on the staff, is indispensable in accomplishing the mission of the staff."

Scott was interviewing for a nursing job in the fledgling research laboratory's Health Division. Likely contributing to any job interview jitters was the fact she was a Black woman seeking a professional position in the Jim Crow South, a reality she acknowledged in a 1952 article published in the *American Journal of Nursing*:

> A casual observer might think that a Negro nurse could have any available position for which she qualified in this unique town. But such is not the case. The town is new, yes, and there are no traditions. But the old patterns of segregation and discrimination are the same. However, because of a large number of highly trained, liberal employees at the laboratory that have come from other sections of the country, the objections to the employment of a Negro nurse on an unsegregated basis are less formidable than they would be in most Southern towns.

As she noted, Oak Ridge's more cosmopolitan and highly educated population may have been more accepting of a Black woman than most Tennessee towns and workplaces. Scott's actual experience at ORNL was more of a mixed bag. She saw acceptance and also prejudice.

Scott reported she encountered no discriminatory attitude among the Health Division staff. Among patients, the "highly trained personnel whom I cared for often displayed a feeling of warmth." Some white employees "seemed amazed" at her nursing skills. Others wanted nothing to do with her and were provided with white nurses.

Her descriptions of her experiences at ORNL were published soon after she arrived at ORNL, in the publications *Industrial Nursing* and *National Negro Health News*, and ultimately in the 1952 *AJN* article. On one occasion she was asked "where I had learned to write so well!"

Doris Belle Scott. Image credit: ORNL

At the lab, Scott oriented newly hired Black employees to its health services and carried out special health programs. She led the planning for National Negro Health Week and joined an effort with the local union to improve living accommodations for African American workers.

A meningitis outbreak in the late 1940s hit Oak Ridge's Black community particularly hard. Scott worked with local agencies and the Oak Ridge hospital to share health information with the area's Black families. A blood screening event she helped organize with the local Citizens Health Committee made up of African American citizens drew 1,500 participants.

"The need for health education in the Negro community was obvious to these groups, and they readily agreed to help in any way that they could," Scott wrote.

President Harry Truman, perhaps prompted by the *AJN* article, in 1952 appointed Scott to serve on the Industrial Health Section of the President's Committee for Health, one of just 10 professionals invited to join the panel.

Scott, a native of Gainesville, Georgia, lived in Knoxville and according to her employment record also had a connection to Knoxville College, a historically Black school. She did her pioneering work at ORNL until 1955, when she married and moved to Cincinnati, Ohio, where she resided until her death in 1996.

President Harry Truman selected ORNL nurse Doris Scott to serve on the Industrial Health Section of the President's Commission for Health. The committee's purpose was to inventory and study national health needs and related education. Image credit: ORNL


From left, J.S. Felton, Doris Scott and G. Williams, October 1949. Image credit: ORNL

Welcome to Research Insights

Atoms for applications: quantum technologies of the future

ORNL Review is pleased to present the second issue of Research Insights, a collection of research articles from our scientific and technical staff. Research Insights was created to provide a cross-cutting view of the exciting research programs taking place at ORNL, with each issue addressing an overarching theme.

This issue reflects the recent movement to leverage the quantum mechanical nature of materials to revolutionize information sciences, understand fundamental material processes, and provide novel methods of measurement, computing, and analysis.

The relevant quantum technologies are still in their infancy, and a great deal of research and development will be required to exploit the potential of this emerging frontier. In recent years, ORNL has grown a substantial program in this area with a diverse set of applications, including the recent creation of the Quantum Science Center. Articles in this issue showcase a sampling of ORNL quantum science and technology research programs, including neutron applications to quantum materials research, biological imaging using quantum light, development of novel systems for quantum information science through manipulation of atomic defects, and control of topological phases in quantum materials using light. We kick off this issue of Research Insights with an article that chronicles the history of quantum science at ORNL leading to the creation of the Quantum Science Center.

We hope you enjoy this sampling of the exceptional work being done by ORNL researchers.

New Frontiers in Quantum Science

T. S. Humble, M. A. McGuire

Quantum Science Center

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INTRODUCTION

Our enhanced mastery of quantum mechanics has advanced our understanding of nature and expanded the tools we use to build increasingly powerful technologies. This newfound knowledge was recently extended to the frontier of information to yield a discipline now known as quantum information science (QIS), a domain that harnesses the phenomena of quantum superposition, tunneling, entanglement, and uncertainty to increase information processing speed, accuracy, and efficiency.

Emerging quantum technologies have demonstrated significant new capabilities for computing, communication, and sensing, thus advancing how we store and transfer quantum information. Technologies that could arise from quantum science represent a highly anticipated opportunity for American economic competitiveness and sustained scientific leadership for the 21st century. This includes advancing scientific discovery, ensuring energy efficiency, and meeting emerging challenges in national security.

To this end, the National Quantum Initiative Act of 2018 directed the US Department of Energy to establish five National Quantum Information Science Research Centers (NQISRCs) tasked with strengthening quantum science and technology while developing the next-generation workforce to ensure American leadership in this critical domain. The Quantum Science Center (QSC) at Oak Ridge National Laboratory (ORNL) is one of the NQISRC focal points committed to the discovery and innovation of new quantum materials, quantum sensors, and quantum computing applications. The QSC has built on ORNL's past investments in quantum materials, quantum sensing, and quantum computing to align our institutional strength with the unique capabilities brought by partnering with a network of nine universities, three companies, and four national laboratories. Our partners include Caltech, ColdQuanta, Fermi National Accelerator Laboratory (Fermilab), Harvard University, IBM, Los Alamos National Laboratory, Microsoft, Pacific Northwest National Laboratory, Princeton University, Purdue University, University of California–Berkeley, University of California–Santa Barbara, University of Maryland, University of Tennessee–Knoxville, and University of Washington.

The QSC integrates a broad research agenda to realize three long-term scientific goals. The first goal is to develop topological qubits that are resilient against noise and errors as a key building block for technologies. Promising topological electronic materials will be transitioned into prototype devices to demonstrate the unique statistical signatures of topological quantum computing. Currently, we are synthesizing and characterizing candidate materials while honing the fabrication and device physics needed to control these systems.

The second goal is to directly characterize and discover quantum states using novel quantum sensors. We are currently developing an underground test station at Fermilab that can be used to probe topological devices while protecting them from the known effects of cosmic radiation. Sensing techniques developed across our partner institutions will then be used to characterize the candidate material samples described above, as well as the new techniques for dark matter searches.

The third goal is to demonstrate the applicability of quantum computing for scientific discovery and innovation. Research in hardware development, software control, and algorithm design are being integrated to build efficient, accurate quantum simulation platforms. Key application areas include quantum chemistry, materials science, neutrino physics, and discrete optimization, and we plan to demonstrate the end-to-end development of quantum computing systems for scientific discovery.

BACKGROUND

QIS represents information by using the quantum state, a concept born from quantum mechanics. The quantum state encodes information as a superposition of mutually orthogonal outcomes that is manipulated to perform sophisticated calculations. In practice, realizing quantum bits, or qubits, requires the control of individual atoms, electrons, and composite "quasiparticles" that result from interactions among electrons inside materials. These qubits must also be entangled together, and this requires exquisite physical control of the quantum state.

Entanglement produces nonclassical mixtures of basic quantum states that provide the power of quantum information. This highlights a key challenge for QIS: quantum states are delicate and must be carefully protected to persist long enough to be useful for storing information. This challenge is addressed by minimizing uncontrolled interactions between the particles and their environment, keeping the system at very low temperatures to reduce thermal noise and unwanted excitations, and actively monitoring for errors during operation.

A certain class of quantum states, known as topological states, has a natural degree of protection built into them. Topological states are found in materials in which the topology of the electron wave functions produces quasiparticles governed by non-Abelian anyon statistics. They are intrinsically robust because the quantum states are distributed over multiple objects separated in space. As a result, the coherent state survives

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local disturbances at individual sites. The QSC is dedicated to advancing these ideas for topologically protected quantum information by developing suitable materials and new ways of interrogating their topological and quantum natures.

Alongside the development of these new topological qubits, other types of qubits are being used to demonstrate new platforms for quantum computing. Qubits based on atomic and photonic systems are available through our partners at IBM and ColdQuanta. We are working together to show how these quantum states can be entangled and manipulated to perform computation. These systems have already demonstrated tens to hundreds of qubits, which is sufficient for small-scale demonstrations of quantum computing.

As quantum computing scales up to larger systems, there is strong theoretical evidence that there will be significant speedups in the time-to-solution and efficiency of computation for many scientific challenges. This includes calculating the quantum states of complex materials systems, chemical dynamics, nuclear physics, and high-energy physics, among many other domains. However, the presence of uncontrolled noise in these devices leads to errors in operations, so the QSC is developing methods to mitigate these errors to improve the efficacy of current devices for performing scientific calculations. Key challenges include characterizing the unknown sources of noise, as well as programming the devices to mitigate against these errors.

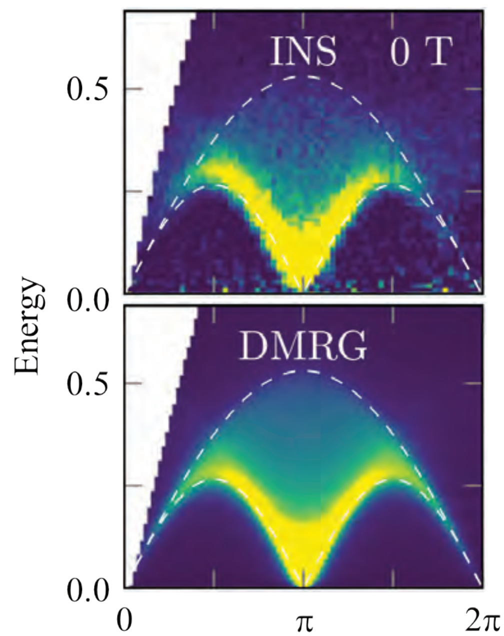

Figure 1. Energy and momentum dependence of excitations in the quantum magnet Cs_2CoCl_4 from inelastic neutron scattering experiments and density matrix renormalization group theory. This information can be used to measure the entanglement of quantum magnetic states. (Credit: Laurell et al. [6])

RESULTS

Over its first year and a half, the QSC has made remarkable progress toward the goals of understanding and harnessing quantum entanglement in topological materials, advancing robust quantum computing algorithms, and developing enhanced quantum sensors.

Progress in topological materials includes key advancements in (1) quantum magnets and quantum-spin liquids, which can host naturally entangled states that can be very insensitive to electrical disturbances, and (2) topological electronic materials, which can host elusive but exciting non-Abelian anyons that are particularly promising for QIS.

Ruthenium trichloride—$RuCl_3$—is believed to be a quantum-spin liquid hosting the correct physics to support long-range quantum entanglement and anyons. Neutron scattering and complementary tools are being used by the QSC and its collaborators to better understand the magnetism, excitations, and thermal transport in this important material [1–4]. Demonstrating entangled quantum states and identifying individual anyons presents a major challenge, because by definition, they are shielded from interactions (i.e., measurements). This is especially true in quantum-spin liquids.

Beyond any single material, the QSC is developing new measurement techniques that apply to the broader field of quantum magnets and quantum-spin liquids. This includes new neutron scattering techniques for quantifying the entanglement of quantum spins in a crystal (see Figure 1), as well as new designs for devices that can detect anyons in quantum-spin liquids using thermal currents flowing along the edge of material, encircling the potential anyons [5].

QSC has also made important progress in materials and techniques of topological electronic materials. Effort here is focused on topological superconducting systems that may host non-Abelian anyons as excitations. These systems combine topology and superconductivity within a single material or at the interface of topological and superconducting materials.

Specifically, a templated growth technique was developed to grow topological materials as thin films on freestanding graphene monolayers [7]. This provides a novel way to interface quantum materials with one another, and perhaps more importantly, it provides a method for carefully controlling geometrical features of topological materials that can trap anyonic states.

Detecting such states is a key challenge, and important progress has been made in this direction for topological superconductors, just as it has for quantum-spin liquids. The QSC is developing a new transport measurement technique that employs scanning tunneling microscopy to identify anyons trapped in superconducting vortices based on how current hops through a vortex lattice [8].

A different form of quantum sensing under development within QSC is based on magneto-optical techniques for characterizing materials surfaces. These methods use the magneto-optical Kerr effect (MOKE) to probe birefringence in a material's surface, and we have combined this with quantum optical sources to enable measurement beyond the classical limit. Our work has used interferometric readout for low-temperature MOKE measurements [9]. Figure 2 shows equipment set up for experiments in ORNL's quantum optical laboratory.

Alongside our work in characterizing materials, we are building new sensors to discover exotic states of matter, such

Figure 2. ORNL's quantum optical laboratory houses our continuous-variable quantum computing system and MOKE characterization experiments [9]. (Credit: Claire Marvinney, ORNL)

as axion candidates for dark matter. These yet-to-be-observed particles harbor a physics believed to mirror topological magnetic insulators, which hints at the deeper connection of how QIS underlies the fabric of our universe.

The QSC is building in-house platforms based on atomic and photonic qubits for tailoring the design of quantum simulations. For example, following up on previous support from ORNL's Laboratory Directed Research and Development funding, the QSC is developing a customized ion-trap quantum simulation device and a novel continuous-variable quantum optical system. The sophisticated control and measurement of these quantum computing test beds will be enabled by our in-house software development for quantum programming. In collaboration with partners at Microsoft, we are implementing a new standard for compiling programs to quantum computers, enabling a team of quantum computer scientists to test new methods for mitigating noise and errors that may arise during quantum computation.

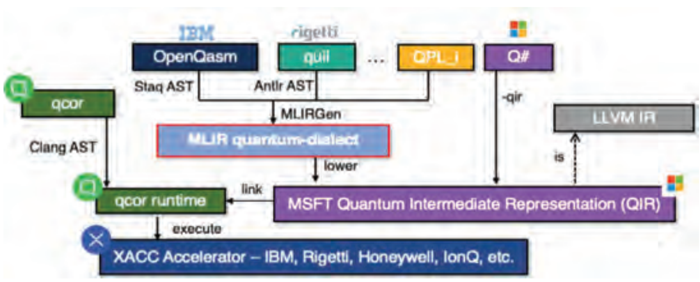

Figure 3. The QSC translates quantum algorithms for scientific applications into machine instructions for quantum computers using a hierarchy of intermediate representations. (Credit: McCaskey and Nguyen [11])

As we develop applications using quantum computing, we emphasize the scientific domains of chemistry, materials science, nuclear physics, and high-energy physics. For example, we are developing new algorithms for calculating the excited electronic states of complex molecules by using the quantum computer to minimize energetic configurations [10]. We translate these algorithmic methods into low-level machine instructions using novel intermediate representations tuned to quantum computers [11]. Figure 3 shows how quantum algorithms developed for use with world-leading supercomputers work together as quantum applications.

CONCLUSIONS

The QSC offers a remarkable platform from which ORNL and its partners can accelerate innovation in QIS. A key objective to achieving each of these goals is to transition fundamental concepts into working demonstrations. The QSC structures this development through what we call the innovation chain, which highlights the intersections between different individual efforts. For example, in our development of quantum simulation platforms, we have integrated work on ion-trap devices with cryogenic electronic control systems. These new platforms are validated against numerical simulations run on the high-performance computers at the Oak Ridge Leadership Computing Facility (OLCF)—namely, Summit—to test the quantum algorithms prior to hardware.

To ensure the success of QSC, the state-of-the-art experimental and computational facilities offered by DOE User Facilities must be leveraged to perform this work. This includes the Spallation Neutron Source, High Flux Isotope Reactor, and National High Magnetic Field Laboratory, the Center for Nanophase Materials Sciences, and the Center for Integrated Nanotechnologies, as well as the OLCF.

QSC's enduring success relies on the development of a diverse, capable workforce trained in the equipment and concepts necessary for QIS research. We are actively engaged across the laboratories, universities, and industrial partners to enable the next generation of scientists and engineers through our postdoctoral student association, our annual Quantum Summer School, and our monthly Meet-a-QIST-Expert series. We also hold an annual competition to award the most promising new research ideas from our QSC postdocs for independent development. More information is available at www.qscience.org.

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Expanding the Quantum Frontier with Neutron Scattering at ORNL

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INTRODUCTION

Neutrons are an irreplaceable scientific resource for quantum materials research, empowering researchers to see "where the atoms are and what they do" in materials [1]. Oak Ridge National Laboratory (ORNL) is the home of two world-class neutron sources, the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS). Using these facilities, researchers have gained significant insights into technology-related quantum phenomena such as high-temperature superconductivity, giant magnetoresistance, entanglement, and topologically nontrivial spin textures. New instrumentation at the planned third source, the Second Target Station (STS) at SNS, will benefit from an increased peak brightness of long-wavelength neutrons and recent advances in neutron optics, sample environments, and computing. This will allow future researchers to fully exploit the neutron's exquisite sensitivity to magnetism and low-energy excitations. STS will enable scientists to study and model new quantum materials at the earliest stages of their discovery, examine exotic interfacial states in detail, and investigate the effects of more extreme external conditions. ORNL's world-leading neutron scattering capabilities allow researchers to expand the quantum materials frontier, with long-term goals including new and improved dissipation-free electronic devices, energy-efficient power transmission, faster computation, and secure communications.

BACKGROUND

Quantum materials hold promise to be at the heart of advances in technology in the fields of computing, quantum information and encryption, sensors, and energy applications. This is no longer the realm of theory and speculation; we are entering a quantum frontier in which quantum materials will be found in the devices we encounter in our daily lives. As articulated in a recent US Department of Energy workshop report, "Quantum materials possess exotic physical properties that arise from the interactions of their electrons, beginning at the atomic and subatomic scales where the extraordinary effects of quantum mechanics cause unique and unexpected behaviors" [2]. The properties and behaviors of quantum materials cannot be explained using classical or even semiclassical descriptions. At the atomic scale, the laws of quantum mechanics govern the behavior of spin, charge, and angular momentum degrees of freedom. The collective behavior of electrons subject to these interactions is what allows quantum properties to emerge in materials. High-temperature superconductivity, magnetic materials both with and without long-range order, and topological insulators are all examples of quantum materials in which the many-body physics of electrons yields materials whose behavior is quantum in nature. Quantum devices can be used to encode information for more secure communications, their quantum bits (i.e., qubits) can be used in computation, and they can make power transmission more stable and efficient. However, to use quantum properties, quantum states must be effectively read, manipulated, and preserved, which requires a fundamental understanding of the underlying quantum behavior of these materials. Fortunately, there is a probe that can quantify the spatial and energy landscape of quantum materials: neutron scattering.

The neutrons used for this research are produced at SNS, HFIR, and STS. These neutrons travel at speeds ranging from a few hundred meters per second to more than tens of thousands of meters per second. This broad spectrum of speed makes the neutrons useful for studying materials and their underlying quantum states. Neutron scattering also allows researchers to study materials within complicated sample environments such as high-field magnets, pressure cells, and at very low

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temperatures. These tools allow scientists to tune quantum states while using neutrons to track how they change at length scales on the order of several nanometers and at energies comparable to the coldest temperatures of interstellar space. The neutron also has a magnetic moment that can interact with the magnetic moments of quantum materials. The patterns and energies of the scattered neutrons from quantum materials can identify the quantum ground states and excitations present. The amount of measured scattering can often be quantitatively compared to calculated values that describe these states.

QUANTUM MATERIALS RESEARCH AT SNS AND HFIR

Individual neutron scattering instruments are designed and optimized to study different aspects of materials to provide further knowledge about these systems. Powder and single-crystal diffractometers measure scattered neutrons from materials to determine the locations of atoms in crystal lattices. The neutron's magnetic moment allows researchers to use neutron diffraction to determine the directions of the magnetic moments or spins, their magnitude, and whether magnetic moments form any short-range ordered structure. Diffractometers at HFIR (POWDER) and SNS (POWGEN and NOMAD) can accurately determine the magnetic structures in powder samples. Single-crystal diffractometers can resolve not only the magnitude of the scattered neutrons' momentum transfer, |Q|, as in powder diffractometers, but also its direction relative to the crystallographic directions of the material being studied. The TOPAZ and CORELLI single-crystal diffractometers at SNS and the WAND² and DEMAND diffractometers at HFIR are all routinely used to study the chemical and magnetic structures in quantum materials.

Single-crystal diffuse scattering has become an increasingly valuable diffraction technique for materials research. Novel properties of quantum materials are often tied to short-range correlations rather than their long-range average structures because of chemical doping or competing interactions, for example. Structural disorders are nearly ubiquitous in high-temperature cuprate superconductors that support dissipation-free energy transport and in colossal magnetoresistance materials that display ultrasensitivity to magnetic field changes. Additionally, short-range magnetic correlations are often seen in frustrated magnetic systems, some of which may host a magnetic entangled state that can be used for quantum computing. CORELLI and TOPAZ, the time-of-flight diffractometers at SNS, have gone beyond the traditional crystallography that solves the average structures of materials. The instruments rapidly collect both strong and weak scattering signals continuously over a large momentum space that contains multiscale microstructural information. Recently developed data analysis algorithms can map the experimental data into real-space correlations without an a priori structural model. One example is the 3D magnetic pair distribution function (3D m-PDF) technique, shown in Figure 1 [3], which shows how an atom magnetically interacts with its neighbors in a spin glass system and whether their magnetic moments prefer to align in the same direction (red color, positive correlation) or in the opposite direction (blue color, negative correlation). Furthermore, researchers are using high-performance computing and machine learning algorithms to analyze the large datasets from exotic magnetic

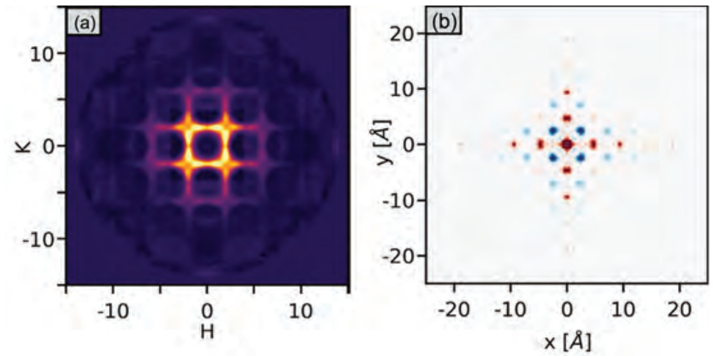

Figure 1. (a) Magnetic diffuse scattering pattern in reciprocal space collected at CORELLI and (b) the real-space magnetic correlation from Bixbyite ($Fe_{1.12}Mn_{0.88}O_3$) using the recently developed 3D m-PDF technique. These plots show how magnetic ions interact with their neighboring sites in Bixbyite up to a distance of 20 angstroms. (Credit: N. Roth et al.)

materials [4]. These advanced instrumentation and computation techniques can help researchers extract short-range and average microstructural information from technology-relevant quantum materials.

Longer wavelength neutrons can be used in small-angle neutron scattering (SANS) measurements to examine correlations across longer length scales. The general-purpose SANS (GP-SANS) instrument located at HFIR measures the correlations of materials with distances between 10 and 5,000 angstroms. This makes the instrument especially useful in characterizing superconducting materials. Magnetic fields do not uniformly penetrate superconductors. For Type II superconductors, magnetic flux penetrates as a series of quantized vortices that interact to form a vortex lattice with a characteristic length scale well matched to SANS measurements. The vortex lattice was recently examined using the GP-SANS instrument at HFIR for the proposed topological superconductor UPt_3. Topological superconductors have specific properties of interest in quantum computing applications. Figures 2a–2c show how this vortex lattice evolves as a function of temperature at a fixed magnetic field in UPt_3 [5]. By developing further understanding of this field

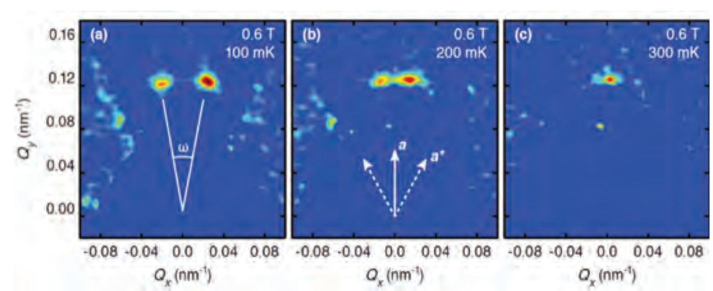

Figure 2. SANS diffraction pattern measured for $UPt3_2$ as a function of temperature for a fixed applied magnetic field. (Credit: Avers et al.)

and temperature dependence, researchers could determine that time-reversal symmetry is not obeyed in the bulk of this superconductor. This has implications for how the topological properties of this system could be used in quantum devices.

Inelastic neutron scattering, or neutron spectroscopy, measures the change in neutrons' energy when they interact with materials. Neutron spectrometers can measure how much energy a neutron deposits within a sample or how much it removes from a sample. These scattering processes can generate lattice excitations (i.e., phonons) or magnetic excitations (i.e., spin waves). For quantum materials, these magnetic excitations can also be present without any long-range ordered magnetic structure. In these cases, the neutron scattering measurement directly measures the excited quantum states of the underlying system. Instruments at SNS (cold neutron chopper spectrometer [CNCS], HYSPEC, SEQUOIA, and ARCS) and HFIR (polarized, thermal, and cold triple-axis spectrometers) are specialized in these types of neutron spectroscopy measurements for the examination of quantum materials. These instruments are optimized to perform measurements over different ranges of energy transfer and with different ranges of energy resolution to provide a complete picture of the dynamics in quantum materials.

The study of quantum systems based on effective spin half-degrees of freedom has recently expanded. These systems are based on ions of Ru, Ir, Yb, and Co, in which coupling between the spin and orbital degrees of freedom leads to an effective angular moment of one-half in the system. In the case of $Yb_2Si_2O_7$, the CNCS instrument was used with a high-field magnet to survey excitations as a function of magnetic field at a temperature of T = 0.05 K (Figure 3) [6]. In this system,

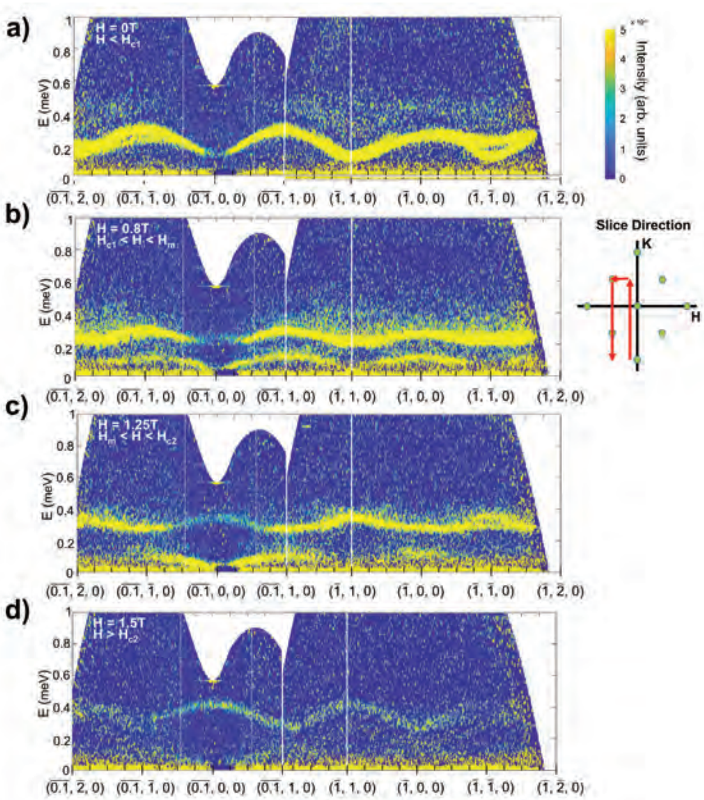

Figure 3. Single-crystal inelastic neutron scattering cross sections as a function of different directions in reciprocal space. Each panel shows the dispersing magnetic excitations throughout reciprocal space. The panels illustrate how the spectrum evolves as a function of applied magnetic field. (Credit: Hester et al.)

the Yb ions pair up to form a cooperative quantum dimer. The applied magnetic field can then drive the energy of this ion pair to lower and lower values until it reaches zero. At this point, the magnetic excitations will have gone through a Bose-Einstein condensation. This critical point in the spectrum can be further studied to understand how the field sensitivity in these systems can be used in quantum-based devices.

New instruments at SNS and HFIR are being designed to push the boundaries of quantifying quantum materials using neutron scattering. The future DISCOVER powder diffractometer will quickly measure systems with short-range structural and magnetic order in various sample environments. This will allow neutron scattering measurements to quantify short-range magnetic order in quantum materials at the earliest stages of their development. The MANTA instrument at HFIR is a new triple-axis spectrometer that will provide an unprecedented flux of neutrons to examine details of magnetic excitations in quantum materials under extreme conditions of low temperature, high magnetic field, applied pressure, or more than one of these conditions simultaneously. Together, MANTA and DISCOVER will provide capabilities to expand our understanding of the frontier of quantum materials.

QUANTUM MATERIALS RESEARCH AT THE SECOND TARGET STATION

STS is also being designed with instruments to look further into the quantum frontier of materials. The source characteristics of STS complement the strengths of the First Target Station (FTS) and HFIR. The STS source will provide cold neutrons with 25 times brighter peak flux than FTS. The lower operating frequency of STS (15 Hz vs. 60 Hz at FTS) will also provide a broader range of neutron wavelengths in a single-source pulse. The high peak brightness of cold neutrons and the broader wavelength band at STS will enable transformative capabilities, such as the ability to study smaller samples, to perform time-resolved studies, and to investigate hierarchical architectures in detail. STS will have the capacity to support a total of 22 instruments that will take advantage of the latest developments in high-resolution optics, instrument design, and neutron-spin manipulation to allow data to be obtained much faster and with higher precision than any other neutron scattering facility in the world.

Six of eight instruments in the initial STS suite are designed to accelerate quantum materials research. The instruments will require a sample volume that is one order of magnitude less than that used by current neutron scattering instruments. This will allow neutron scattering measurements to direct the materials discovery process. For example, the single-crystal diffractometer PIONEER (Figure 4a), will be the world-leading single-crystal neutron diffractometer because of its capability to measure tiny crystals (0.001 mm^3, i.e., x-ray diffraction size) and thin films (10 nm thickness). This in turn will allow for regular measurements of pressure-induced quantum states and examination of exotic magnetic states at surfaces and interfaces in thin films. The CENTAUR SANS instrument (Figure 4b) is being designed to accommodate both small-angle diffraction and inelastic measurements. This multimodal approach allows for experiments to quickly change course as data are examined. With state-of-the-art spin-manipulation optics, many instruments

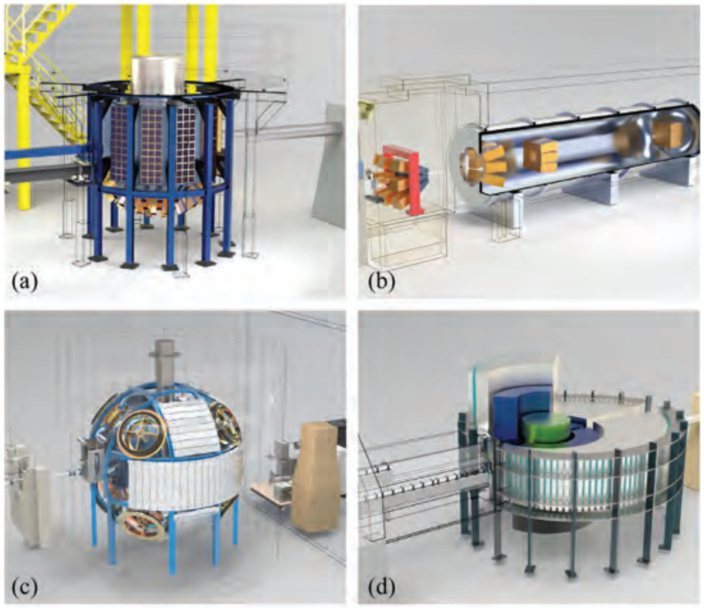

Figure 4. Four of the eight initial instruments of STS. (a) PIONEER single-crystal neutron diffractometer, (b) CENTAUR SANS instrument, (c) CHESS direct-geometry chopper spectrometer, and (d) VERDI powder diffractometer. (Credit: Jill Hemman, ORNL)

at STS will take full advantage of polarization analysis techniques. Notably, CHESS (Figure 4c) and VERDI (Figure 4d)—both focused on magnetism research—will provide the unique polarization analysis capacity over a large momentum transfer Q range to solve structures and dynamics, respectively, from complex magnetic materials. CHESS is also designed to employ the repetition rate multiplication mode [7], so it can measure a sample with multiple energies per neutron pulse. This capability, coupled with the high flux of its moderator and unprecedented detector coverage, will allow CHESS to access different energy scales, simultaneously increasing measurement efficiency.

CONCLUSIONS

Quantum materials are becoming part of everyday life as they are being embedded in new technologies and energy applications. Neutron scattering provides an ideal probe to understand these emerging materials' quantum states and structures. SNS and HFIR will continue to drive the research community toward a more complete understanding of the underlying physics of quantum systems through neutron diffraction, SANS, and neutron spectroscopy measurements under standard and extreme sample environment conditions. STS will provide new instrumentation to further push these boundaries of measurement of quantum states by providing the capabilities to measure smaller samples faster and with greater precision. These new instruments will accelerate the discovery process for new quantum materials, thus providing a bright future of quantum research for neutron scattering at ORNL.

IMPACT

The world-class neutron scattering instruments at SNS and HFIR are contributing to the study of quantum materials by measuring and quantifying long- and short-range ordered magnetic structures, as well as their excitation spectra. ORNL staff members and researchers from around the world use these instruments to further understand quantum materials. Characterization of these materials helps advance the fields of computing, quantum information and encryption, sensors, and energy applications. The quantum frontier will be further explored, with the new instruments being built at HFIR and SNS, as well as the new instrument suite being developed for the STS at the SNS.

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Biological Imaging Using Ultralow Quantum Light

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INTRODUCTION

Imaging offers a direct means to visualize how complex systems function. By analyzing one image or a series of images, one can learn not only critical information about where molecules or metabolites are located within cells or complex environments, but also how they change over time. The most commonly used imaging modality for biological systems relies on illuminating biological samples with a chosen color of incident light and subsequently collecting a different color of emitted light, typically fluorescence, at spatial locations across the sample region. An image is thus a spatial map of the florescence intensity and therefore localizes the presence of fluorescent molecules, providing an optical means to visualize biological systems. Although this conventional approach is straightforward, it has obvious limitations. Specifically, it applies only to biological systems or molecules capable of producing fluorescence, or it requires the addition of exogenous fluorescent labels. The addition of labels can destroy or disturb biological functions in the worst cases.

To overcome these limitations, advanced imaging techniques known as nonlinear optical (NLO) microscopies have been developed that use two, three, or more incident light bursts lasting only a few millionths of a billionth of a second (~20 fs = 20 x 10^{-15} s) to induce multiple light–matter interactions on a singular molecular species [1]. These NLO imaging methods offer various unique contrast mechanisms to visualize biological systems without the use of labels. For instance, one can design the optical fields to leverage molecular vibrations or light absorption characteristics as *intrinsic* contrast in complex samples. These tools are especially useful for accessing biological systems, and they function at the smallest molecular and subcellular levels based on their capability to extract chemical and molecular information, compatibility with biological samples, and flexibility to incorporate complementary imaging modalities.

However, the strong light fields resulting from the use of multiple ultrashort pulses can cause photodamage and perturbations to cells, thereby preventing prolonged imaging of living systems. An example of such photodamage is illustrated in Figure 1, in which acquisition of a single image using an NLO modality based on molecular vibration as contrast caused substantial cell damage in 10 s, even while demonstrating light levels some four orders of magnitude lower than typical [2]. The photodamage and phototoxicity represent a long-standing, severely limiting, omnipresent challenge to bioimaging using light. Consequently, there is often a trade-off between maintaining the integrity of the biosystem and simultaneously extracting useful information through any optical imaging modality. To address this challenge, new techniques capable of operating under *dramatically* lower light levels are needed to enable truly noninvasive analyses and detection of many key biological processes. Emerging quantum-based imaging approaches using entangled photons (discussed below) have shown unique potential to surpass these limitations and barriers.

BACKGROUND

Two-photon fluorescence (TPF) microscopy is by far the most widely applied NLO imaging modality. By absorbing two photons successively, a molecule undergoes an electronic transition from its initial ground state to an electronic excited state. The subsequent relaxation transition results in the emission of a fluorescence photon with energy *greater* than either of the individual incident photons. Because neither of the two photons creates an excited state on its own that can degrade molecular targets, photobleaching and toxicity are not as problematic as in conventional fluorescence microscopies. Typically, light in the near infrared (NIR) spectral range is used for TPF microscopy because most biological materials have either weak or absent absorption in the NIR region, so light is not strongly scattered. Consequently, these photons can penetrate deep (several 100s of μm) into the systems of interest. Combined with reduced light scattering, the interaction of several photons with the same species provides a mechanism for 3D sectioning, allowing the acquisition of complete spatial images of complex systems with molecular and subcellular resolution. Because any given photon pair used to create the excited state is a random combination of two individual photons, the resulting TPF signal scales with the squared intensity of the incident photons. This means that generation of an appreciable signal necessitates a very-high-intensity burst of light, making photobleaching and photodegradation a persistent problem.

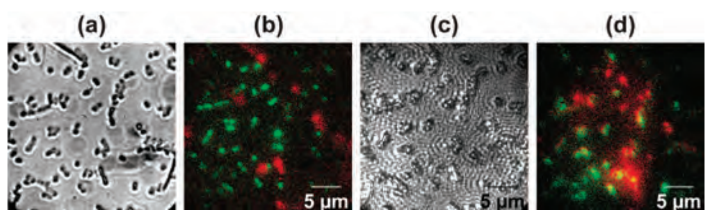

Figure 1. (a) Brightfield and (b,d) composite TPF images acquired from *Pantoea* sp. YR343 cells stained with live/dead assay dyes before and after acquisition of an image based on a vibrational contrast in 10 s (c), which led to more dead cells manifested by the appearance of more red spots in (d) than those seen in (b). (Credit: Uvinduni Premadasa, ORNL)

What if, instead, we employ correlated "twin" photons—or entangled photons—which is a specific form of quantum

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light, for TPF microscopy? Such a quantum entangled photon pair possesses unique properties such that the color of one of these photons and its arrival time at a molecule, and its other characteristics can be used to predict the precise color, arrival time, and characteristics of the other photon in the pair. Thus, such an entangled photon pair is considered to be a single quantum object, because absorption of the twin photons occurs simultaneously. This has a peculiar effect, in that the corresponding entangled two-photon response now scales linearly with the intensity of the incident entangled photons. This contrasts with the squared intensity dependence described above for the classical counterpart [3]. This entangled two-photon response can be either fluorescence or absorption, a direct measure of the attenuation of the incident entangled photons by a sample under study, which is called entangled two-photon fluorescence (ETPF), or entangled two-photon absorption (ETPA) for fluorescence or absorption modalities, respectively. This linear intensity means that the same level of ETPF or ETPA signal can be realized with a substantially lower intensity of entangled photon pairs. Thus, ETPA/ETPF methods can be leveraged as a fundamental mechanism to solve the long-standing challenge of photodamage and phototoxicity in bioimaging.

This linear scaling of entangled two-photon responses has been experimentally observed for over two dozen molecular species, including flavins and flavoproteins, using up to 10 orders of magnitude lower light levels than needed for corresponding classical two-photon measurements. This unprecedented signal enhancement stems from a single parameter known as the ETPA cross section, a unique property dictated by both the molecule itself and the quantum nature of entangled photons. This contrasts fundamentally with classical two-photon absorption, in which the corresponding two-photon absorption cross section is a solely molecular property independent of the classical light field. This remarkable signal enhancement of entangled two-photon responses has enabled acquisition of ETPF images from a spatially heterogeneous microcrystalline film using a photon flux that was six orders of magnitude lower than that needed for the corresponding classical TPF image [4]. Although the extent of this enhancement and even its feasibility as a novel NLO spectroscopic and imaging tool currently remains a subject of debate—not surprising for an emerging research field—the unique properties of this quantum light approach hold unprecedented potential to revolutionize bioimaging to provide noninvasive and nondestructive visualization of biosystems under in vivo conditions. This article briefly describes ongoing research in this emerging field and highlights the approach to push the barriers of ETPF imaging for biological systems.

RESULTS

Our research on this topic centers on combining adaptive pulse shaping with entangled photon generation and application. Specifically, this ongoing research is aimed at developing a new entangled two-photon microscope with several unique capabilities, including group delay dispersion compensation (i.e., controlling the spread of distinct frequency components of the entangled photon light in time), and optimization of entangled photon generation and its resulting two-photon absorption response. This dispersion compensation is key, because so-called virtual electronic states, which exist only during the presence of the optical pulse, serve as a kind of stepping stone for the two-step electronic transition of an ETPA event. Given that these states are short-lived, the presence of dispersion in the pulse means that only a fraction of the available entangled photon pairs will arrive within the lifetime of the virtual state(s), and the remainder are wasted. Dispersion compensation becomes even more important when a thicker nonlinear crystal is used for entangled photon generation based on a so-called spontaneous parametric down-conversion (SPDC) process, in which a single-pump photon is divided into identical twins known as signal and idler photons. Historically, these terms have been used to distinguish the photons in a pair with high and low energies, respectively. For a given pump intensity, a thicker crystal corresponds to a brighter SPDC source capable of producing a greater flux of entangled photon pairs, but it also causes more pronounced dispersion problems that must be addressed. Conveniently, a bright SPDC source allows for control over the pulse characteristics using pulse-shaping methods developed at ORNL, where the deleterious dispersion contributions can be corrected. In view of the significant challenges, this effort has been conducted in two phases. Phase I is focused on pump pulse shaping to optimize entangled photon generation and its resulting ETPA response, which is built on the team's expertise in coherent pulse shaping, in combination with the well-established approaches for entangled photon generation and utilization. In Phase II, this work will be followed by adaptive pulse shaping of the entangled photon pairs for optimal ETPA responses.

Pump pulse shaping for entangled photon pair generation. Although SPDC sources based on femtosecond (fs, 1 fs = 10^{-15} s) pulsed and continuous wave (CW) lasers have been demonstrated by numerous research groups, the optimal spectral and/or temporal characteristics of pump lasers for efficient entangled photon generation, especially for desired ETPA/ETPF responses, remains unexplored. It was predicted recently that pump pulse shaping can enable effective engineering of the quantum state of SPDC and enhancement of ETPA [5], but no experimental verification has been reported so far.

Our ongoing effort is based on a mode-locked femtosecond laser, which produces ~50 fs pulses with a central wavelength at ~810 nm (NIR) at a repetition rate of 82 MHz. The laser output is frequency-doubled using a first beta barium borate (BBO) nonlinear crystal to generate pulses centered at ~405 nm (blue color light). This NLO process relies on sequential interaction of two NIR photons to generate a new photon with twice the energy of the input NIR photon energy. The resulting blue laser light is separated from the NIR light using two mirrors capable of reflecting only the blue light and is directed into a so-called 4*f*-pulse shaper built from a transmission grating, a folding mirror, a focusing optics, and a 2D spatial light modulator (2D-SLM), as illustrated in Figure 2. The grating spatially separates individual frequency components analogous to the color separation in a rainbow. These components are focused onto the Fourier plane using a cylindrical mirror. The Fourier plane is a unique location where the pulse shaper can adjust the phase (i.e., delay characteristics) and amplitudes (i.e., light levels) using an array of independently controllable liquid crystal elements (i.e., pixels). By focusing each of the individual frequency components in the pump pulse onto each element along the horizontal direction, one can independently modulate the properties of each color in the pulse. In principle, this allows for the generation of *any* arbitrary pulse shape, such as those shown in Figure 2. The shaped pump pulses are subsequently directed to a second nonlinear BBO crystal to generate entangled photon pairs based on the SPDC process described above. Compared to the entangled photon generation and the application based on fixed-pulse or CW laser output, this pump pulse–shaping capability offers a unique opportunity to explore the correlation between pump pulse shape and entangled photon characteristics to identify an optimal pulse shape for generating the most efficient SPDC source and optimal ETPA/ETPF responses.

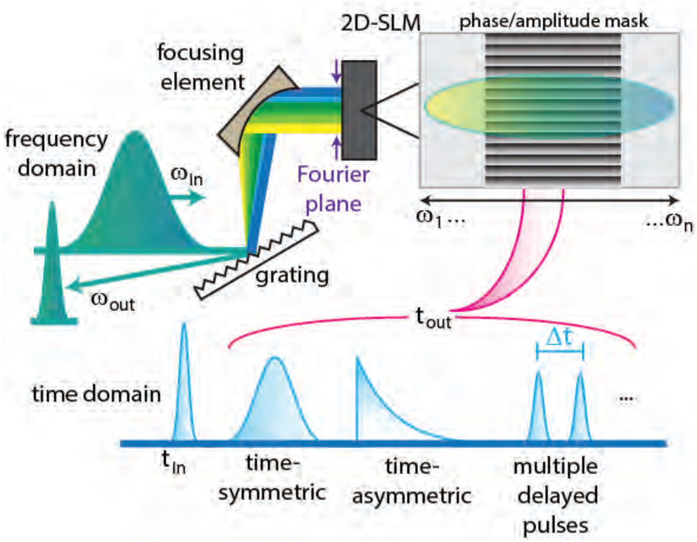

Figure 2. Schematic of simplified operating principles for pump pulse shaping based on a 2D-SLM pulse shaper with a folded geometry, and examples of several pulse shapes that can be generated. (Credit: Benjamin Doughty, ORNL)

Adaptive pulse shaping of entangled photon pairs. As noted above, the ETPA response is extremely sensitive to the excitation characteristics of the entangled photon pairs, so its optimization offers an effective means to tune such a response for *any* given molecule. In Phase II, an adaptive pulse-shaping capability will be developed to modulate the entangled photon pairs for optimal ETPA response. This effort is further motivated by recent observations that the ETPA cross section of a selected molecule depends strongly on spectral bandwidth of the entangled photon pairs, and the observed dependence was further found to vary with the type of nonlinear crystals used for SPDC processes. This observation is also consistent with recent theoretical predictions regarding the enhancement of ETPA efficiency upon optimal pulse shaping of entangled photon pairs [5]. However, several key questions remain to be addressed. What are the desired spectral and/or temporal characteristics of entangled photon pairs for optimized ETPA responses? Are the desired characteristics dependent on molecular species? How can one achieve optimized ETPA cross section for any molecule? Adaptive pulse shaping of entangled photon pairs offers a powerful means to search and optimize a vast parameter space and represents a unique approach to fit the microscope to the problem and not to design molecules to fit the microscope.

Although the design of such an adaptive pulse shaper is in principle identical to that shown in Figure 2, all the optical components must be replaced with those designed for the NIR wavelength of the entangled photon pairs. Even more importantly, to enable modulation of both signal and idler photons simultaneously, major modifications are needed to accommodate both beams on separate vertical regions of a same 2D-SLM and to modulate them independently.

Successful implementation of this adaptive pulse shaping of entangled photon pairs must overcome several challenges. Beside the losses caused by inclusion of complex optical components in the signal and idler photon beams, which can be many orders of magnitude weaker than the pump pulse, it is extremely important to minimize or ideally eliminate the loss of either a signal or an idler photon. The loss of a photon reduces or even eliminates a quantum advantage owing to the undesired contribution from classical two-photon absorption events [6–7]. This critical requirement means that independent control of the signal and idler photons must ensure that survival or cessation occurs only in a pair-wise manner. A further challenge arises from the large parameter space that must be explored to find an optimal set of parameters for the largest ETPA response. A crucial question is how to search for the optimal value of any given parameter or a set of such optimal values for the entire parameter space for any chosen molecule. This question might be addressed using ORNL's artificial intelligence and machine learning methods that have yet to be explored.

Imaging the spatial and temporal dynamics of gene expression in the rhizosphere. As an integral component of this ongoing project, critical validation for the unique capabilities of the quantum light microscope will be benchmarked by imaging complex biological systems using known methods. These labeled species must be capable of producing appreciable levels of fluorescence emission with the entangled photon pairs, as the quantum light intensity is many orders of magnitude lower than that typically used for classical experiments. Therefore, gene expression processes will be imaged in the rhizosphere using transcriptional reporters. The rhizosphere is the area below ground that is influenced by the presence of the plant root and includes the complex community of organisms that lives within this zone of influence. Importantly, the rhizosphere is not uniform; rather, it is composed of many microenvironments with differing chemical and physical characteristics, depending on the local community composition and organization, as well as temperature, hydration, and oxygen levels in the environment. Community members respond to these local conditions by changing their behaviors and physiologies such that the same species may express a different set of genes, depending on its location in the community. For this reason, measuring the spatial and temporal dynamics of gene and protein expression in the context of a complex biosystem is a key step to unraveling and predicting gene functions and cellular behavior. The system's spatial heterogeneity and prolonged gene expression process make it particularly suitable for assessing the noninvasive, nondestructive capability of the new entangled two-photon microscope.

A flavin-based transcriptional reporter (i.e., iLOV) was selected for this validation for multiple reasons. First, LOV domains bind flavin mononucleotide as an ultraviolet/blue light–absorbing chromophore, which emits green fluorescence upon photoactivation, as shown in Figure 3. Second, the feasibility of an iLOV-based reporter for such quantum light imaging has been demonstrated by recent ETPF measurements on flavin-binding proteins. Through ETPF imaging in space and time, we expect that the gene expression patterns in complex rhizosphere systems can be directly visualized at high frequency for extended times with little disturbance to the biosystem. Observing the spatial and temporal dynamics of microbial gene expression on intact plant–microbe communities with little perturbation can provide new insights into microbial gene functions and will help elucidate how complex rhizosphere communities are established and maintained.

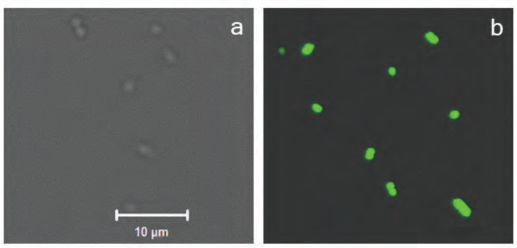

Figure 3. The bacterial strain *Pantoea* sp. YR343 carrying a transcriptional reporter plasmid. The green fluorescence observed in the cells in (b) comes from expression of iLOV fluorescent protein in response to promoter activation. Control *Pantoea* sp. YR343 cells (a) carrying an "empty" plasmid that does not have a promoter to produce the iLOV fluorescent protein. (Credit: Jennifer Morrell-Falvey)

CONCLUSIONS

The remarkable enhancement of ETPA responses has enabled NLO imaging with substantially lower levels of light than currently feasible, and thus it holds promise to solve the long-standing challenge of overcoming photodamage and phototoxicity in bioimaging-related science. This article discusses the ongoing quest in this emerging field and highlights the unique potential afforded by combining adaptive pulse shaping to achieve optimized ETPA response for *any* chosen molecule species. Critical validation of the unique capabilities of this quantum light microscope necessitates specifically selected and designed biological systems, which are currently under development.

IMPACT

This research addresses the significant challenges inherent in prolonged, real-time imaging studies by substantially reducing light intensities relative to current technology. These technological advances will be broadly applicable and will enable fundamental understanding of complex biological processes occurring in living plants and microbial systems in real time.

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Taming Atomic Defects for Quantum Functions

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INTRODUCTION

Alice needed to go down a rabbit hole to reach Wonderland. But for us, the best way to reach the quantum wonderland [1] may mean never leaving it in the first place. All materials, regardless of how trivial they are, are governed by the rules of quantum mechanics at the atomic level. However, in most cases, these fundamental properties are diluted into a classical picture in the macroscopic world. To harness these hidden properties, we usually look at so-called "quantum materials," which expose the quantum mechanical nature of matter to our view at macroscopic scales. At this scale, the quantum functions show up in various forms such as superconductivity or nontrivial electronic band topology. On the other hand, by simply staying in the atomic scale, we may be able to tame more fundamental quantum functions like entanglement and single-photon emission.

Single atoms provide an ideal system for utilizing fundamental quantum functions. Their electrons have well-defined energy levels and spin properties. Even more importantly, for a given isotope—say, 12C—all the atoms are identical. This creates a perfect uniformity that is impossible to achieve in macroscopic-size quantum systems. However, herding individual atoms is a very difficult task that requires trapping them by magnetic or optical means and cooling them down to temperatures in the nanokelvin range [2]. On the other hand, the counterpart of single atoms—the single defects—may be as good as atom-based quantum systems if not better. These defects, also referred to as quantum defects, possess the favorable energy, spin, and uniformity properties of single atoms and remain in their place without the help of precisely tuned lasers. While the number of usable isotopes is set, the combinations of defects and their host material are practically limitless, giving us the flexibility to create precisely designed and controlled quantum systems. Furthermore, as we tame these defects for the quantum world, we bring about transformative opportunities to the classical world in forms such as ultradense electronic devices and precise manufacturing.

In this Research Insight, we introduce some of our recent work on precisely controlled creation and manipulation of individual defects with a scanning tunneling microscope (STM). We also discuss possible pathways for utilizing these capabilities for the development of novel systems for quantum information science (QIS) applications such as quantum information processing and ultrasensitive sensors.

BACKGROUND

Atomic-scale defects such as vacancies and substitutions (i.e., dopants) play an important role in controlling the electronic properties of materials. Today, most electronic devices rely on the sheer concentration of defects rather than the individual defects themselves. Utilizing single defects for classical or QIS applications faces two challenges. First, the defects are usually buried deep in the bulk, limiting access to the defect and making it hard to understand the exact defect structure. Second, creating the desired defect structures requires the capability to manipulate individual atoms with atomic precision.

The first challenge has been mostly addressed with the advent of 2D materials over the last two decades. These materials bring every single atom and defect within the range of optical and electronic probes. Furthermore, some of the most popular 2D materials—hexagonal boron nitride [3] and transition metal dichalcogenides (TMDs) [4], for example—have already shown us that they have defect structures that act as single-photon emitters (SPEs) [5] at room temperature. However, 2D materials host many native defects that come in different variations and are randomly distributed in the 2D material. Therefore, despite the tremendous efforts to identify the exact structure of SPEs, it is still not clear which defect(s) are responsible.

While being equally important, the second challenge has been tackled far less than the first one. The randomness in defect distribution takes us back to today's electronic devices, for which only the defect concentration for large-scale devices can be safely counted on. If the defects are to be used individually in ultradense electronic devices or as qubits in QIS applications, their precise structure, location, spatial separation, and environment should be observed and controlled with atomic resolution. STM is one of the few techniques that can address this challenge, as it is equipped with advanced imaging, spectroscopy, and manipulation capabilities, all at the individual atom level (Figure 1). These capabilities make it possible to

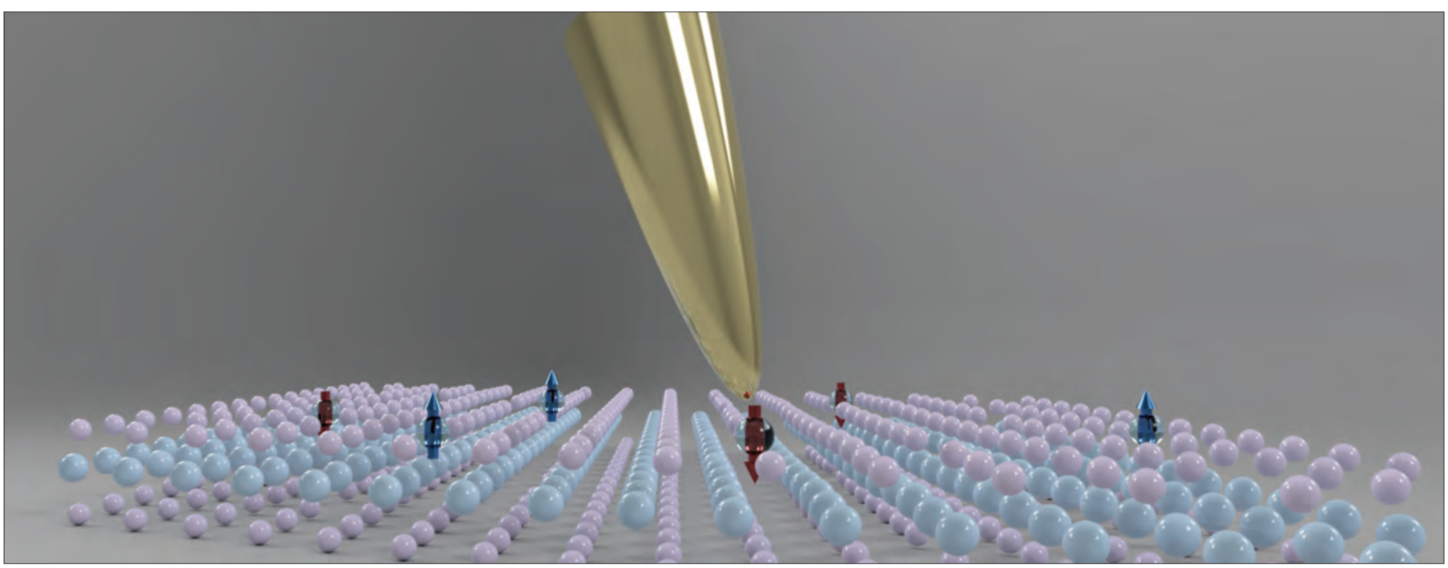

Figure 1. STM builds on the fundamental principle of quantum tunneling; allows imaging, spectroscopy, and manipulation, all at the individual atom level; and offers the capability of taming individual defects for deterministic quantum functions. For instance, STM can be used to manipulate the spin orientation (red and blue arrows) and location of individual defects (clear balls) in the crystal lattice of 2D materials (pink and blue balls). (Credit: Saban Hus, ORNL)

identify individual defects and create or manipulate the desired defect structures by moving atoms into a chosen geometry [6].

Our current research aims to address both challenges. We use STM to identify host material and defect structures, link structures with the desired functionalities, and develop techniques to individually modify defects to gain new functions.

RESULTS

Development of single-defect memory devices. Since the development of the first integrated circuits, the size of basic electronic devices (e.g., transistors, resistors, memory units) has been scaling down. In this race to miniaturization, the ultimate goal has been reaching a scale at which a single atom controls the device's function. We achieved this goal by creating a two-terminal memory unit, also known as memristor, which can switch between 0 and 1 states by moving a single gold atom in and out of a vacancy defect in atomically thin TMD layers [7]. These memory devices are composed of monolayer 2D materials sandwiched between two gold electrodes [8]. In this work, we first identified and characterized the defects of the 2D material with STM. Then we positioned a gold STM tip at the individual defect locations and used it in contact mode to act as the top electrode of the nanoscale device. We demonstrated that a single chalcogenide vacancy constitutes the active region of the device. Under a proper electric field created by the STM, a gold atom from the electrodes can be moved in and out of this vacancy, which reversibly tunes the local electronic structure between metallic and insulating characteristics, respectively (Figure 2). In this work, we demonstrated that quantum defects can be modified with atomic precision to create the smallest classical memory devices.

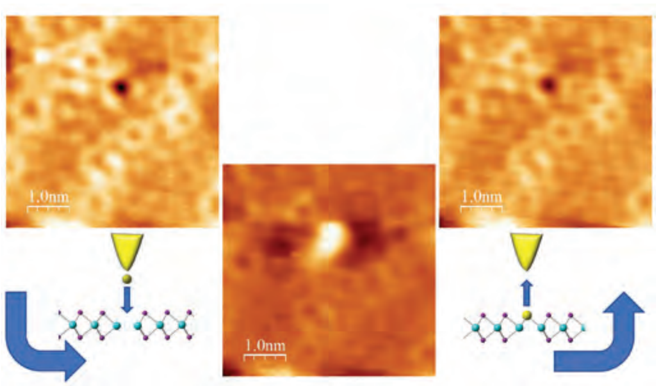

Figure 2. Individual vacancy defects in TMD monolayers can be filled with gold atoms with field-induced atom migration from the tip. This reversible process alters local electronic states between insulating and metallic characteristics, creating binary states (labeled 0 and 1) of atomic size memories. The method is applicable to many other quantum defect–metal atom pairs and can be used to create designed defect structures. (Credit: Hus et al.)

The ongoing pursuit is utilizing these skills to create and test novel magnetic defect structures. Multiple theoretical studies indicate that the defects in 2D materials can host spin-polarized electronic states due to strong spin–orbit coupling [9]. Experimentally, STM studies have already confirmed the existence of a large ~250 meV splitting between spin-polarized defect states of sulfur vacancies in WS2 [10]. Filling these vacancies with different magnetic or nonmagnetic atoms may create even more pronounced and tunable spin states. The functionality of these defects is similar to spin-polarized magnetic adatoms on metal surfaces [10], which are seen as possible candidates for qubits and spintronic applications. But magnetic adatoms are extremely mobile on metal surfaces and require very low temperatures to stabilize and manipulate. On the other hand, most defects in 2D materials are spatially and energetically stable at room temperature, making them more amenable to experiment and application.

STM manipulation allows us to go beyond randomly distributed defects and create deterministic ones. For instance, defect structures with longer spin coherence time can be designed, built, and tested. Similarly, defect pairs with a controlled spatial separation can be created to observe the interaction between their spin states. Furthermore, our multiprobe STM capabilities [11] enable us to tune this interaction by using one of the probes as a gate between two defects.

3D defect engineering. Defect manipulation in 2D materials is also possible beyond monolayer films. Using STM, we can identify the 3D lattice locations of selenium vacancy (VSe) defects near the surface of layered pentagonal TMD-PdSe2 [12]. Furthermore, we can reversibly switch the defects between neutral and negatively charged states and trigger their migration within the lattice, by using STM both as a movable electrode and characterization probe.

In STM, a small bias voltage (typically <2 V) is applied between tip and sample to create and measure the tunneling current between them. When the STM tip is very close to the surface, this bias acts as a gate voltage and locally bends the electronic bands of the semiconductor materials. If the semiconductor has a defect state within the band gap and close to the Fermi level, this band bending may push the defect states across the Fermi level. As a result, the defects can be switched between neutral and charged states. Crossing the Fermi level creates a step in the tunneling current that is displayed as charging rings in dI/dV maps. The band-bending effect is reduced as we get farther away from the tip. Therefore, the defects at the lower layers display smaller charging rings. By measuring the size of these rings, we can identify the depth of the defect with high precision.

Compared to hexagonal TMDs, the unique pentagonal lattice of PdSe2 has weaker covalent bonds and holds lower barrier energies for vacancy migration. This makes it possible to both "write" and "erase" an atomic defect from a particular lattice site by applying slightly higher voltage pulses (~2.0 V) than typical bias (Figure 3). Once the desired vacancy geometry is created, the vacancies at the top layer can be filled with substitute atoms to add new functionalities. Furthermore, the vacancies in the underlying layers can be utilized to modify the local charge and energy landscape.

Magnetic end states in atomically precise graphene nanoribbons. Graphene is one of the original quantum materials in which the electrons behave as massless Dirac fermions. In its pristine 2D form, graphene does not have a band gap, which limits its direct utilization in QIS applications. However, lattice defects, including the edges, break graphene's structural

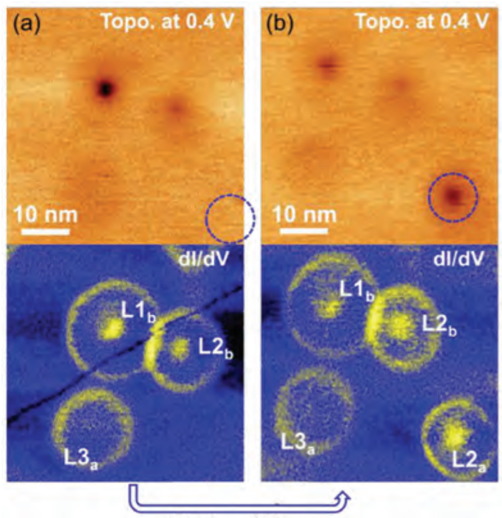

Figure 3. Individual vacancy defects can be written and erased (not shown) by applying voltage pulses to the surface of a layered material, PdSe2. The size of charging rings around the defects can be used to identify the depth of the defect. (Credit: Nguyen et al.)

symmetry and create a local environment where the electronic structure is significantly modified. In the 1D form of planar graphene, namely graphene nanoribbons (GNRs), an electronic band gap is opened due to quantum confinement, and nontrivial electronic states can emerge. In their atomically precise form, these nanoribbons are of great interest for QIS applications due to their spin-polarized edge states; coupled spin centers; and highly tunable electronic, optical, and transport properties [13].

GNRs are typically synthesized with metal surface–assisted chemical reactions, leaving us with nanoribbons on a noble metal substrate. However, the metallic surface states of the substrate strongly couple with the electronic states of the GNR and suppress its distinctive properties. Transferring the nanoribbons to insulating substrates is also challenging because any alteration in its atomically precise edges will modify the electronic states of interest. Therefore, using a nonmetallic substrate for synthesis is highly desirable. Using specifically designed precursor molecules, we synthesized precise GNRs on the surface of rutile titanium dioxide (TiO_2), which is a large band gap insulator [14].

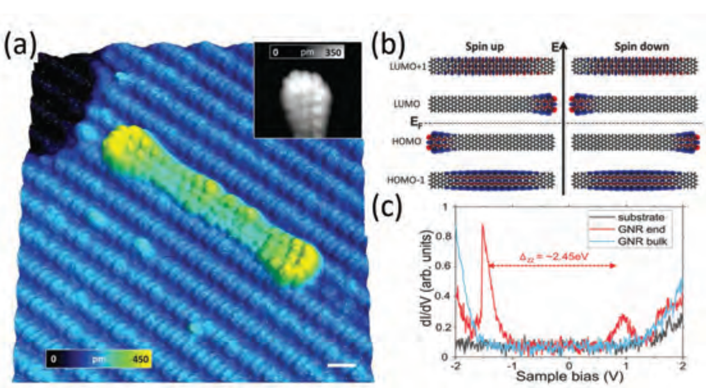

Figure 4. (a) STM image of atomically precise armchair GNR on rutile TiO2 surface. (b) Nanoribbons have zigzag ends with coupled spin centers. (c) The insulating substrate enables observation of magnetic end states with a 2.45 eV splitting. (Credit: Kolmer et al.)

Our STM studies on these nanoribbons confirmed the formation of planar armchair GNRs with well-defined zigzag ends as well as the decoupling of their electronic states from the substrate.

STM measurements (Figure 4) confirmed the existence of magnetic zigzag end states spatially separated by semiconducting nanoribbons. We observed the theoretically predicted spin-1/2 end states with an exchange gap of 2.45 ± 0.10 eV (Figure 4c). Electronic states at the ends of such a narrow nanoribbon thus give rise to a pair of nonlocally entangled spins. When combined with recent developments in microwave transmitting scanning probe microscopy techniques, these electronically free-standing GNRs could enable qubit initialization, logic gate operation, and readout. STM manipulation of these nanoribbons and probing their transport properties with multiprobe STM can lead to the creation and testing of complex quantum circuits.

CONCLUSIONS

Advanced, atomic-scale imaging, spectroscopy, and manipulation capabilities of STM make it possible to assemble multiple atoms into a chosen geometry so that defects can be created at will. STM thus offers a transformative approach to tame defects for QIS applications. Combining STM manipulation with in situ synthesis and characterization capabilities, we are able to create atomic defects and interfaces that deliver novel quantum states, such as entangled spins, single-photon emissions, and atomic memories. These quantum defects enable the creation of emerging qubits and memristors based on graphene, TMDs, and other 2D materials. Our research focuses on determining the host lattice–defect pairs, identifying suitable states for hosting quantum properties, creating these defects in a controllable manner, experimentally verifying the properties of these systems, and uncovering the fundamental physics responsible for these properties.

IMPACT

Atomic defects provide a system that combines the environmental isolation necessary to maintain the coherence of quantum states with the ability to access and manipulate the states via electrical, magnetic, and optical probes. With proper utilization of these defects, we can create quantum states deterministically as well as control interactions and conversions of these states. This capability paves the way for QIS applications such as new ultrasensitive sensors in which quantum systems' extreme sensitivity to external perturbations is utilized, or quantum computing where quantum entangled and coherent ensembles are used for the physical representation and processing of information to tackle problems divergently complex for classic computers..

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Light-Induced Topological Phase Transitions in Atomically Thin Quantum Materials

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INTRODUCTION

Topological materials have their electronic properties robustly protected against local perturbation and hold great promise in diverse quantum applications, including energy-dissipation-less topological electronics and fault-tolerant quantum computing. Controlling topological phases in quantum materials typically requires a change in their structural or chemical properties. Recently, we have developed a new testable theory to predict whether light can be used to tune electronic states and engineer topological phases in atomically thin transition metal dichalcogenides (TMDs) such as monolayer WTe_2 and $MoSe_2$. Through first-principles calculations combined with a tight-binding approach, we predicted that circularly polarized light can trigger topological phase transitions in TMDs. Furthermore, by controlling the intensity of light irradiation, different topological phases can be realized. For instance, increasing the light intensity can drive the quantum spin Hall (QSH) state into the quantum anomalous Hall (QAH) state. The latter state requires no symmetry for protection and provides a more robust platform toward the realization of topological superconductivity. Finally, light can also enlarge the topological nontrivial band gaps in TMDs, making them more experimentally detectable. Our predictive model demonstrates the power of light in tailoring topological phases in atomically thin materials for targeted quantum technologies, and it will enable accelerated experimental discovery of new topological phases that do not exist in equilibrium.

BACKGROUND

Engineering quantum materials with emergent properties on demand is an important aim in modern condensed matter physics, which promises to boost research on future nanodevices and quantum computers [1]. One of the emerging strategies is using light or laser technology [2]. We can obtain information on the structural and electronic properties of materials by electromagnetic radiation (i.e., light); spectroscopy is an example of this kind of technology. Light can also drive materials out of equilibrium and thus allows for hidden phases to be accessed [2]. For example, light can induce or enhance superconductivity [3]; light can also change a material's crystal structure transiently to induce ferroelectricity [4]. To manipulate the electronic band structures in materials, ultrafast laser pulses have been considered. The phenomena in experiments can be elucidated well by Floquet-Bloch theory [5].

Floquet band engineering in materials, which is realized by periodically oscillating electromagnetic fields, provides a way to realize topological phase transitions [6]. Topological phases in materials hold promise for fault-tolerant quantum computing due to the nontrivial edge states that are robust against local perturbations in real space. In 2D systems, two important gapped topological phases are present, namely the QSH and QAH states. The QAH effect does not require any symmetry to be protected, while the QSH effect requires time-reversal symmetry. This means that the QAH effect is basically robust against any disorder, while the QSH effect is robust only against nonmagnetic disorder. Though the QAH effect is very important in condensed matter physics, so far there are only a few successful experimental realizations under limiting conditions such as extremely low temperatures or high magnetic fields [7]. However, as circularly polarized light could break time-reversal symmetry and introduce an effective mass term or spin-orbital coupling in materials, it opens the opportunity to realize and tailor topological phases. This idea of Floquet band engineering has been applied in graphene to induce a sizable nontrivial QAH

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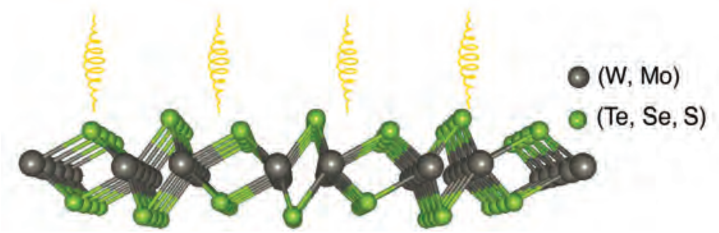

Figure 1. Side view of 1T'-phase TMDs under light irradiation.
(Credit: Kong et al.)

gap in theory, and theoretical predictions were experimentally confirmed as integer anomalous Hall conductance was realized successfully in graphene under light irradiation [8]. Experimental advances in other materials such as Bi_2Te_3 have also resulted in observations of Floquet bands and light-induced band gaps [9].

In our work, using ab initio–based Wannier tight binding methods, we investigated Floquet band engineering in atomically thin TMDs [7], as shown in Figure 1. 1T'-phase TMDs have been reported to host the QSH effect in the ground state and superconductivity by applying a gate voltage or varying the carrier density [10, 11]. The intersection of topology and superconductivity in 1T'-phase TMDs raises the hope for topological or fault-tolerant quantum computing. Our results demonstrate that circularly polarized light can manipulate nontrivial band gaps and induce topological phase transitions in 1T'-phase TMDs.

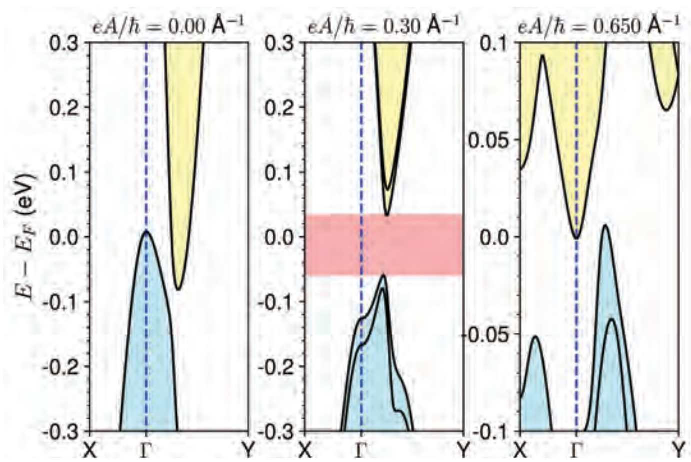

Figure 2. Light-induced Floquet bands in 1T'-phase WTe_2.
(Credit: Kong et al.)

RESULTS

Light can enlarge nontrivial band gaps. As shown in the left panel of Figure 2, without light irradiation, 1T'-phase WTe_2 exhibits the QSH effect but with semimetallic properties, according to our first-principles density functional theory calculations. With light irradiation, the Floquet bands can be split, and the overall band gaps are enlarged; this is good because the topological nontrivial edge states will emerge in the full band gap. With increasing light intensity, the Floquet band gaps decrease again, as shown in the middle and right panel of Figure 2. At finite light intensity, band inversions are not observed in 1T'-phase WTe_2 (also $MoTe_2$), and thus the light-induced QAH effect with insulating properties is not expected. However, if we consider other materials in the 1T'-phase TMDs family (e.g., WSe_2), the light-induced transition from the QSH state to the QAH state could be observed as discussed below.

Light can induce topological phase transitions. A band inversion is a necessary condition for a topological phase transition. In 1T'-phase WSe_2 with light irradiation, band inversion clearly occurs. As shown in the left panel of Figure 3, without light irradiation, WSe_2 exhibits the QSH effect with

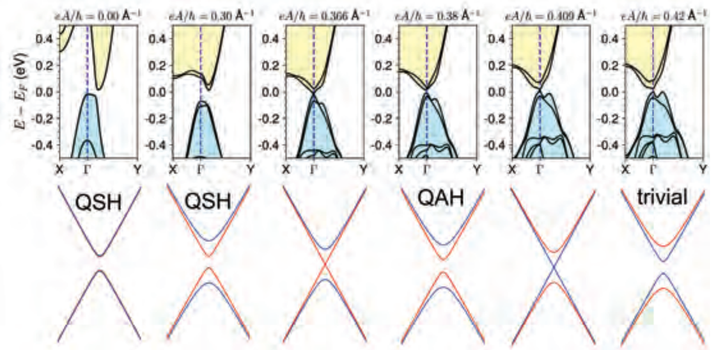

Figure 3. Light-induced Floquet bands and topological phase transitions in 1T'-phase WSe_2 with schematic diagrams.
(Credit: Kong et al.)

double degenerate bands due to both time-reversal symmetry and inversion symmetry. When the light intensity increases, a band splitting can be observed. However, as there is no band inversion, the WSe_2 system preserves the topological properties of the QSH effect but with broken time-reversal symmetry. As the light intensity increases further to 0.366 Å^-1 (third panel from left), there is a band closing point at the Γ point. By continuing to increase the light intensity to 0.38 Å^-1 (fourth panel from left), the band crossing is lifted. Here, we can conclude that there is a band inversion and subsequently a topological phase transition from the QSH to the QAH phase. As discussed above, the QAH phase is a more stable topological phase that is robust against any kind of disorder. Therefore, such a QSH-to-QAH transition induced by light bears potentially significant technological importance. In addition, the light-induced QAH band gap is sizable, and the nontrivial band gap can reach up to 30 meV by tuning the light intensity. As the light intensity increases further to 0.42 Å^-1 (rightmost panel), there is another band inversion occuring, leading to a transition from a topological nontrivial phase to a topological trivial phase.

To confirm the light-induced topological phase transitions, we evaluated the edge states of the light-WSe_2 coupled system as shown in Figure 4. At first, the helical edge states can be clearly observed in the QSH insulating phase (left panel) before the first band inversion. When the light drives the system into the QAH phase (middle panel), the chiral edge state can be observed in the insulating bulk band gap. After the second topological phase transition, a gapped trivial edge state is observed (right panel).

Phase diagrams in the whole family of 1T'-phase TMDs. We also investigated the phase diagrams of the whole family of 1T' TMDs with the chemical formula MX_2 (M = W, Mo and X = Te, Se, S) as shown in Figure 5. We found that light can control the magnitude of the QSH insulating band gap in 1T'-phase

WTe_2 and $MoTe_2$ and can induce the QAH insulating phase in 1T'-phase WSe_2, $MoSe_2$, and WS_2.

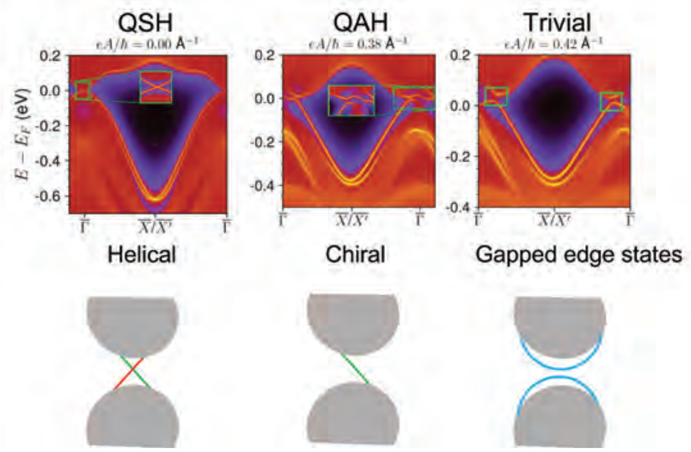

Figure 4. Light-induced edge states from topological phase transitions in 1T'-phase WSe_2. The top images demonstrate the calculations of edge states, and the bottom images show the simplified edge states for guidance. (Credit: Kong et al.)

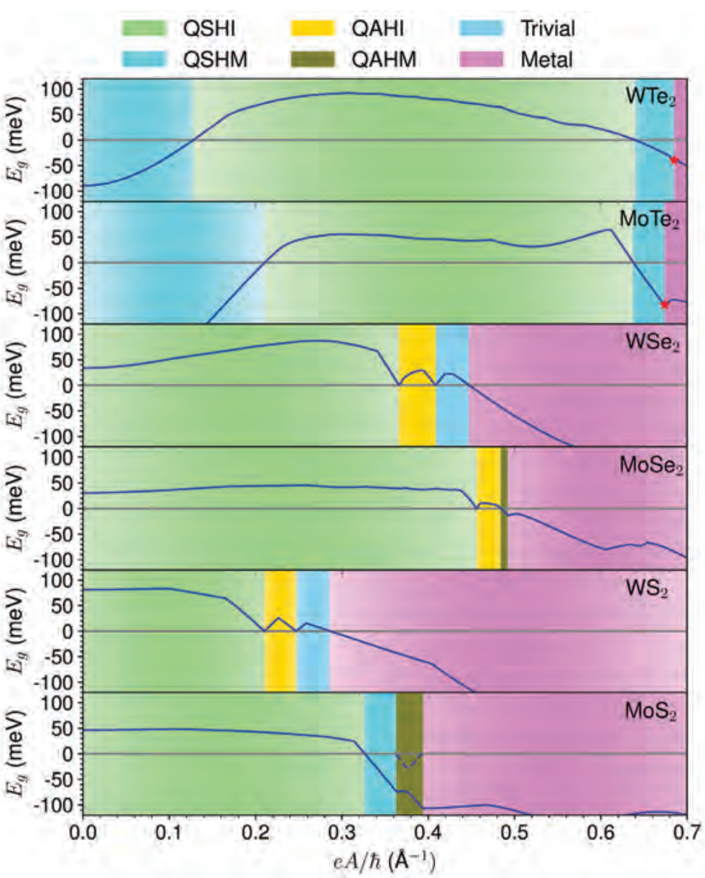

Figure 5. Light-induced phase diagrams in the family of 1T'-phase TMDs with tracking the Floquet band gaps vs. the light intensity. Different colored regions indicate different phases induced by light: QSHI(M) indicates the QSH effect with insulating (metallic) properties, QAHI(M) indicates the QAH effect with insulating (metallic) properties, trivial indicates the trivial insulator phase, and the metal phase indicates the region with complex Floquet bands, which may contain band inversions. The red stars at top right indicate the first band inversions around X points in Te-based TMDs. (Credit: Kong et al.)

CONCLUSIONS

We theoretically demonstrated that periodic light can manipulate the electronic properties of 1T'-phase TMDs based on the Floquet-Bloch theory. Circularly polarized light can break the time-reversal symmetry in nonmagnetic materials and renormalize and/or enlarge the nontrivial Floquet band gaps. Light can also induce different topological phase transitions, especially realizing the desired QAH effect with more robust properties. This work proves that Floquet band engineering is a promising way to tailor quantum materials on demand and provides much-needed guidance for future experimental realizations.

IMPACT

The QAH effect offers a route to topological superconductivity with potential applications in quantum computing. From a general perspective, our study provides a new platform to investigate the out-of-equilibrium physics of light–matter interactions.

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