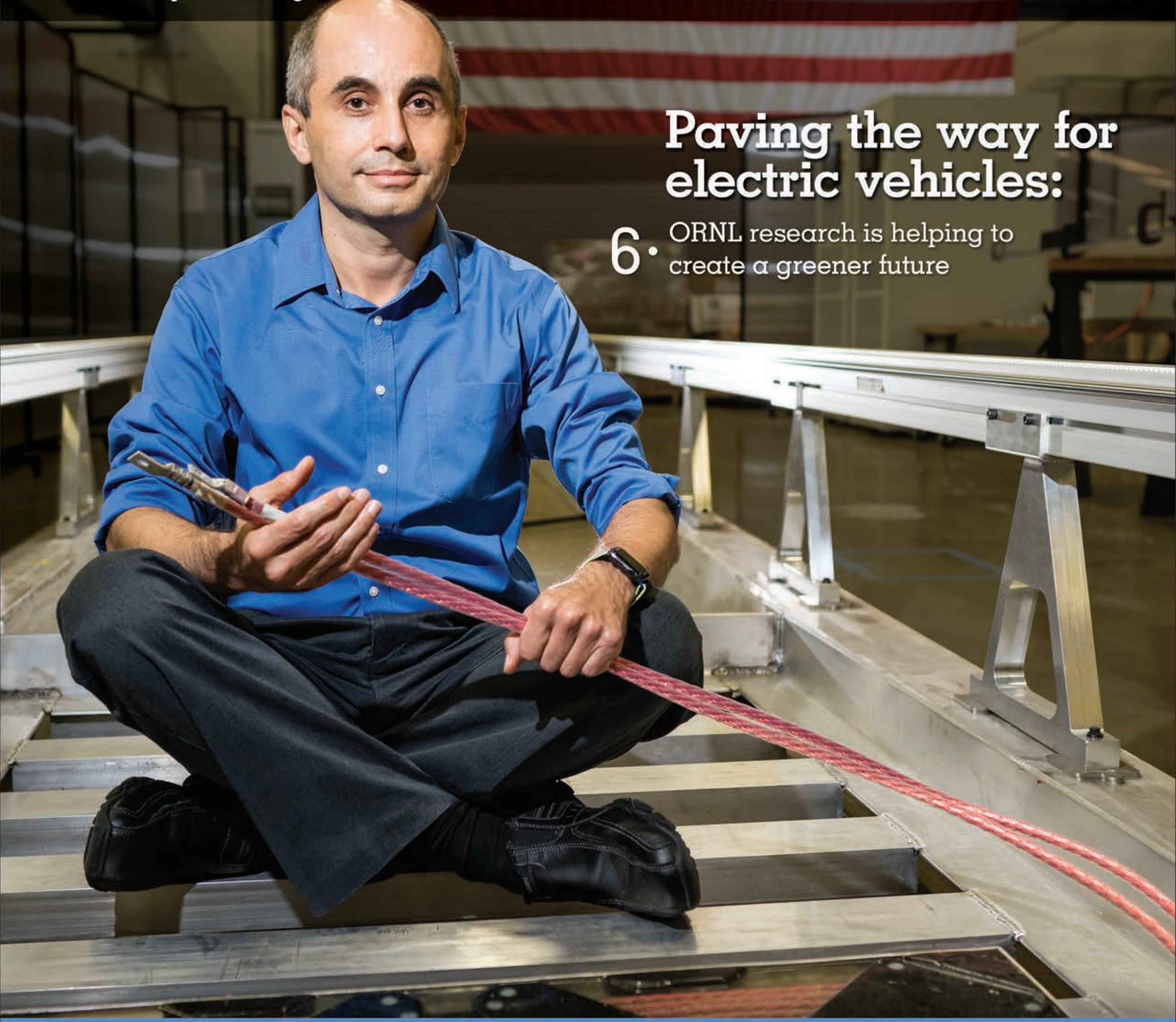
OAK RIDGE NATIONAL LABORATORY

Review



Paving the way for electric vehicles:

OAK RIDGE National Laboratory

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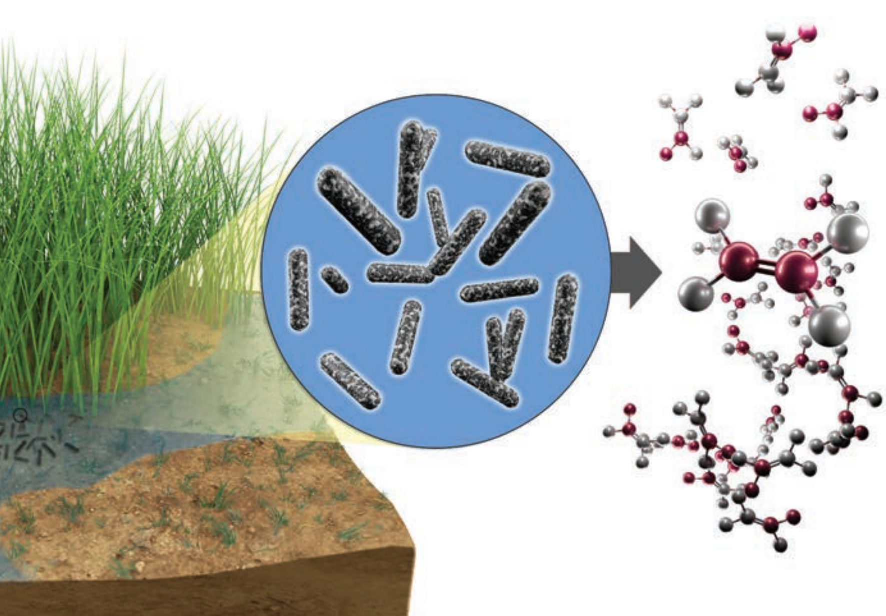


On the Cover

ORNL Vehicle and Mobility Systems Research Section head Burak Ozpineci.
Image credit: Carlos Jones, ORNL

Accelerating electrification to fight climate change

The transportation sector is the leading source of greenhouse gas emissions in the U.S. Vehicles powered by gasoline and diesel fuel release more than 2 billion tons of carbon dioxide each year in the United States. One of the most significant ways to combat global warming is to accelerate the move away from the internal combustion engine and toward electric vehicles.

Governments and businesses are pushing the transition to EVs, but they will need substantial help from the research community. Before consumers will buy tens of millions of EVs, those vehicles need to be more convenient, more reliable, safer and less expensive to operate.

Key to this transition are the batteries used and the speed and efficiency with which they recharge. In this issue of *ORNL Review*, we share what our researchers are doing to improve all aspects of battery technology, making them safer, lighter, more powerful and less expensive (see “Better living through electricity,” page 6). We also examine research that will make vehicle charging both faster and more convenient; in fact, ORNL technology will potentially allow drivers to charge up without stepping out of their cars (see “Going wireless for better vehicle charging,” page 14).

The transition to EVs and other earth-friendly technologies will also require greater access to highly-sought-after materials, most notably a group of 17 elements known as rare-earth metals. Unfortunately, North America does not have major deposits of these metals. ORNL researchers working with the multilab Critical Materials Institute are working to improve this situation in a variety of ways: specifically, by improving the separation of rare earths, finding high-value uses of more common elements, and promoting the recycling of critical materials from used batteries and other discarded consumer products (see “Helping to ensure the supply of critical materials,” page 10).

We are applying ORNL expertise to electrification in other sectors, too. Our Grid Research Integration and Deployment Center, a 52,000-square-foot facility on ORNL’s Hardin Valley Campus, hosts ORNL’s electricity research, including projects to ensure the safety and stability of America’s power grid, promote neighborhood microgrids and develop future battery technologies (see “New center houses ORNL electricity research,” page 16).

Elsewhere in the Review, we introduce our associate laboratory directors, eight research leaders who guide ORNL’s eight primary research organizations. Most of these ALDs have been with the lab less than two years. Their arrival accompanies a major effort at ORNL to ensure the lab’s culture, structure, and priorities position us to best serve the research needs of the Department of Energy and the nation.

This issue of *ORNL Review* also features other ORNL research, including continued contributions to the fight against the COVID-19 pandemic (see “Neutrons map COVID-19 replication mechanism,” page 36, and “Neutrons probe cell membrane defense against COVID-19,” page 38).

Thank you for your interest in the work our researchers are doing to make the country and the world a cleaner, safer place.

Thomas Zacharia
Laboratory Director

Software aids placement of EV charging stations

ORNL researchers have developed a nationwide modeling tool to help infrastructure planners decide where and when to locate electric vehicle charging stations along interstate highways. The goal is to encourage the adoption of EVs for cross-country travel.

The free open-source software, called REVISE-II, takes into account EV growth forecasts, charging technology capabilities, intercity travel trends and driver demographics to help planners fill infrastructure gaps for charging facilities.

By inputting various assumptions, planners can generate scenarios for future charging infrastructure requirements to encourage acceptance of EVs and accommodate growth as more EVs are adopted.

"Providing infrastructure for intercity charging is a necessary step to make EVs fully competitive with conventional vehicles," ORNL's Fei Xie said. "This is a freely available planning tool that takes into account the complexity of intercity travel and helps decision-makers more carefully plan these capital-intensive projects to support a nationwide, electrified future." — *Stephanie Seay*

This summer, supported by critical diagnostics equipment from ORNL, scientists at the Joint European Torus in the United Kingdom are slated to run their first fusion experiments using deuterium and tritium fuel in 25 years. Image credit: EUROfusion

ORNL helps pull data from fusion experiments

Equipment and expertise from ORNL will allow scientists studying fusion energy and technologies to acquire crucial data during landmark fusion experiments in Europe.

ORNL's Ted Biewer led a team that developed diagnostics equipment for JET, the Joint European Torus facility in the United Kingdom, which will allow scientists to better measure and understand the nuclear fusion process.

JET is a test bed for ITER, the international experiment under construction in France that will eventually use deuterium and tritium fuel to demonstrate fusion as a viable, carbon-free energy source.

Deuterium–tritium experiments have been rare in part because tritium is in short supply and challenging to handle. Fusion researchers will use this fuel for the first time in 25 years in JET to maximize fusion performance in anticipation of ITER.

"These JET experiments are historic. It's a rover-touching-down-on-Mars type thing for fusion," said Biewer. — *Kristen Coyne*

The REVISE-II modeling tool developed at ORNL supports decision-making for electric vehicle charging infrastructure development along interstate highways in support of intercity travel. Image credit: Jason Richards, ORNL

New algorithm lowers utility bills

ORNL researchers have designed and field-tested an algorithm that could help homeowners maintain comfortable temperatures year-round while minimizing utility costs.

The algorithm learns over time to keep the home at residents' desired temperature settings while minimizing energy costs and adjusting to environmental conditions, all with no existing knowledge of the building. Results suggest the algorithm could save homeowners as much as 25 percent annually on their utility bills.

"We found it's not practical to try to create a different model for each individual building across a neighborhood or city," ORNL's Helia Zandi said.

"We wanted an algorithm we could apply to different buildings that would automatically learn the characteristics of the environment and how to minimize operating costs while maximizing comfort."

The team's goal is to make the model universal so it can adapt to any system with the least amount of data necessary. — *Matt Lakin*

Scientists found that microbes at the SPRUCE experiment in the Minnesota peatlands are increasing production of methane under warming conditions. Image credit: ORNL

Peatland experiment shows methane growth

Scientists studying a unique whole-ecosystem warming experiment in the Minnesota peatlands found that microorganisms are increasing methane production faster than carbon dioxide production. These results could mean a future with more methane, a greenhouse gas that is up to 30 times more potent than carbon dioxide.

A multi-institutional team examined extensive data from two years of above- and belowground warming at the ORNL-led SPRUCE experiment, including analysis of the species' genome, proteins and metabolism.

"You couldn't see the trend with just the DNA data, but it was apparent when we used high-performance computing to analyze the datasets as a group," ORNL's Chris Schadt said. "Increases in plant productivity under warming and a shift in the vegetation from moss to more vascular plants are providing fuel for methanogenic activity."

The scientists' observations will inform climate models that predict our planet's future. — *Kim Askey*

Building envelope system stores heat, coolness

ORNL researchers have developed a novel envelope system that diverts heat or coolness away from a building and stores it for future use.

Traditional building envelopes, which include roofs and walls, use insulation to reduce heat flow. ORNL's thermally anisotropic building envelope, or TABE, adds thin conductive layers between the insulation. The conductive layers connect to a thermal loop that redirects the heat or coolness to an energy storage system.

Stored energy is then used to heat or cool the indoor space. Sensors and controls determine when to transfer energy between the envelope and the loop to maximize energy savings or peak load reductions.

"Our simulations predicted more than 50 percent energy savings in a residential building," ORNL's Som Shrestha said. "Results from a one-year field demonstration also showed promising results for TABE when used in walls and roofs." — *Jennifer Burke*

An algorithm developed and field-tested by ORNL researchers uses machine learning to maintain homeowners' preferred temperatures year-round while minimizing energy costs. Image credit: ORNL

3D printing can benefit geothermal technology

Additive manufacturing can make the design and production of specialized tools for geothermal energy cheaper and more efficient, according to an ORNL study.

Geothermal is a renewable energy resource that requires specialized tools for drilling in harsh subsurface environments. The tools are typically produced in low quantities at high cost using conventional fabrication.

By using 3D-printing techniques, geothermal companies can take advantage of computer-aided technologies to design tools with enhanced performance characteristics. Those custom parts can then be printed using ORNL's high-strength alloys at a lower cost, especially when printing multiple parts in a single build. The lab's technoeconomic analysis found ample opportunity to lower the cost of geothermal projects while improving system performance using additive manufacturing.

"The study points to the significant benefits of additive manufacturing and provides a roadmap for future work, including the development of new AM feedstocks based on advanced, high-temperature alloys," said ORNL's Yarom Polsky. — *Stephanie Seay*

For more information: https://go.usa.gov/x6FtR

NASA, ORNL team up to create amorphous ice

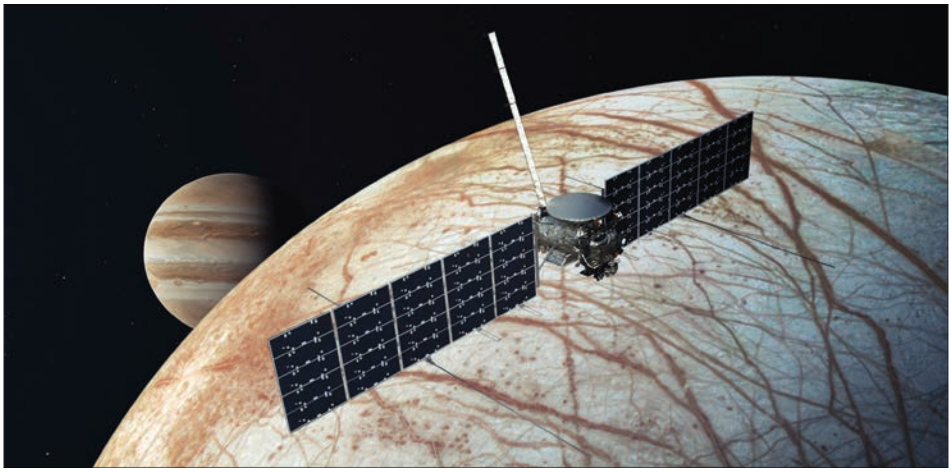
Researchers from NASA's Jet Propulsion Laboratory and ORNL have successfully created amorphous ice, similar to ice in interstellar space and on icy worlds in our solar system. They documented that its disordered atomic behavior is unlike any ice on Earth.

The findings could help interpret data from future NASA missions such as Europa Clipper, which will assess the habitability of Jupiter's moon, Europa.

Using the SNAP instrument at ORNL's Spallation Neutron Source, the scientists replicated the cold vacuum of space and added a few molecules at a time of heavy water to a plate cooled to 25 kelvins to produce amorphous ice. They then used neutron scattering to observe the ice's structural changes at varying temperatures before it transitioned to crystalline ice.

"Amorphous water ice is ubiquitous in the universe, yet isn't well understood. Our data could help understand exotic ice forms in our solar system and beyond," said ORNL's Chris Tulk. — *Paul Boisvert*

For more information: https://go.usa.gov/x6FzQ



Scientists from ORNL and NASA's Jet Propulsion Laboratory studied the formation of amorphous ice like the exotic ice found in interstellar space and on Jupiter's moon, Europa. Image credit: NASA

ORNL licenses AI to General Motors

ORNL has licensed its award-winning artificial intelligence software system, the Multinode Evolutionary Neural Networks for Deep Learning, to General Motors for use in vehicle technology and design.

The AI system, known as MENNDL, uses evolution to design optimal convolutional neural networks — algorithms used by computers to recognize patterns in datasets of text, images or sounds. General Motors will assess MENNDL's potential to accelerate advanced driver assistance systems technology and design. This is the first commercial license for MENNDL as well as the first AI technology to be commercially licensed from ORNL.

Once trained, neural networks can accomplish specific tasks — for example, recognizing faces in photos — far faster and at much greater scale than humans. However, designing effective neural networks can take even the most expert coders up to a year or more.

The MENNDL AI system can dramatically speed up that process, evaluating thousands of optimized neural networks in a matter of hours, depending on the power of the computer used. It has been designed to run on a variety of different systems, from desktops to supercomputers, equipped with graphics processing units.

"MENNDL leverages compute power to explore all the different design parameters that are available to you, fully automated, and then comes back and says, 'Here's a list of all the network designs that I tried. Here are the results — the good ones, the bad ones.' And now, in a matter of hours instead of months or years, you have a full set of network designs for a particular application," said Robert Patton, head of ORNL's Learning Systems Group and leader of the MENNDL development team. — *Coury Turczyn*

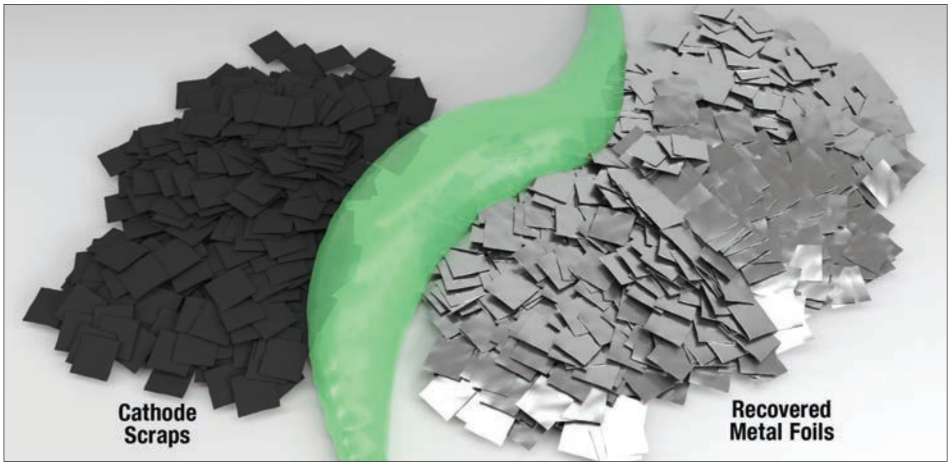
For more information: https://go.usa.gov/x6e2C

Microbial enzyme helps efficiently degrade lignin

In a step toward increasing the cost-effectiveness of renewable biofuels and bioproducts, ORNL scientists have discovered a microbial enzyme that degrades tough-to-break bonds in lignin, a waste product of biorefineries.

When inserted into a bioengineered bacterium, the enzyme helps efficiently convert lignin compounds into a common component of plastics, opening a pathway to transform waste into a commercially valuable biochemical.

"Lignin is a really complicated polymer," said Josh Michener, who led ORNL's research. The polymer, which contributes to the structural rigidity of plants, consists of useful monomer units held together by weak and strong bonds. With lignin making up 20 to 30 percent of plant biomass by weight, breaking the



ORNL's green solvent enables environmentally friendly recycling of valuable Li-ion battery materials. Image credit: Andy Sproles, ORNL

polymer's strong bonds and converting the chemicals they link together into value-added products is necessary to make the production of plant-based biofuels and products economically viable.

Diverse communities of bacteria and fungi perform these processes in nature, but maintaining a mix of so many different microbes in one bioreactor can be tricky. To solve this problem, ORNL scientists at the Center for Bioenergy Innovation want to identify the enzymes that microbes use to degrade specific bonds in lignin and engineer the genes that code for those enzymes into a single organism.

Working toward this goal, ORNL researchers targeted a particularly stubborn bond linking two carbon molecules in a lignin dimer — a unit of two joined monomers — called 1,2-diguaiacylpropane-1,3-diol, or DGPD.

The team used the bacterium *Novosphingobium aromaticivorans*, a microbe of interest in lignin valorization. After identifying and cultivating a mutant *N. aromaticivorans* strain that efficiently degraded the desired linkage in DGPD, the researchers used bacterial genetics and gene disruption techniques to find which enzyme was responsible.

To their surprise, the enzyme they identified — which they named LsdE — had been labeled as a hypothetical protein, meaning its function was unknown.

"No one had seen this kind of chemistry before," Michener said. "There weren't any examples in the literature of a single enzyme that could do this particular transformation." — *Kim Askey*

For more information: https://go.usa.gov/x6Fde

New solvent improves lithium battery recycling

ORNL scientists have developed a solvent that results in a more environmentally friendly process to recover valuable materials from used lithium-ion batteries, supports a stable domestic supply chain for new batteries and keeps old ones out of landfills.

Spent batteries are typically broken down by smelting, an expensive, energy-intensive process that releases toxic gas. The ORNL-developed alternative is a wet chemical process using triethyl phosphate to dissolve the binder material that adheres cathodes to metal foil current collectors in Li-ion batteries. The result is efficient recovery of cobalt-based cathodes, graphite and other valuable materials like copper foils that can be repurposed in new batteries.

"With this solvent, we're able to create a process that reduces toxic exposure for workers and recovers valuable, undamaged, active NMC [nickel-manganese-cobalt] cathodes, clean metal foils and other materials that can be easily reused in new batteries," said ORNL's Ilias Belharouak. — *Stephanie Seay*

Microbe turns waste into valuable chemical

An ORNL-led research team has bioengineered a microbe to efficiently turn waste into itaconic acid, an industrial chemical used in plastics and paints.

In current methods of producing itaconic acid, fungi feed on relatively pure sugars, which can be expensive. In ORNL's demonstration, the team used lignin, a waste product from biorefineries and paper mills, to grow the bacterium *Pseudomonas putida* for potentially cheaper itaconic production.

The trick was to separate the microbes' growth phase from itaconic production using dynamic controls. ORNL designed and deployed a biosensor that triggers the metabolic pathway for itaconic acid production only after the microbes consume all the nitrogen that fuels their growth.

"This technology could provide additional revenue for biorefineries by turning lignin into a high-value chemical," ORNL's Adam Guss said. "One strain achieved nearly 90 percent of theoretical yield during the production phase and could be further optimized. We can also apply these methods to a range of carbon waste streams." — *Kim Askey*

Scientists genetically engineered bacteria for itaconic acid production, creating dynamic controls that separate microbial growth and production phases for increased efficiency and acid yield. Image credit: NREL

Better living through electricity

by Leo Williams
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Energy storage has come a long way since Italian physicist Alessandro Volta stacked pairs of copper and zinc discs separated by brine-soaked cloth, creating the first battery as we know it.

In Volta's achievement, the zinc discs ended up with extra electrons, making them electrically negative. The copper discs, on the other hand, ended up missing electrons, which made them electrically positive. When the two were connected, electrons moving from the zinc back to the copper created an electrical current.

Battery basics have stayed much the same since Volta created that first battery in 1800. Batteries have two sides — or electrodes — separated by an electrolyte. The side with extra electrons (the zinc discs in Volta's battery) is known as the anode, while the side missing electrons (the copper discs) is the cathode. The electrolyte (in Volta's case, the brine) allows charged ions to travel from one side to the other while barring electrons from doing the same.

The details, however, are very different. Instead of copper and zinc, modern batteries rely on lithium, the lightest metallic element and the third-lightest overall. And instead of the weak current created by Volta's pile of discs, modern batteries can hold enough energy to power a vehicle for 300 miles or more.

The future is electric

Electricity powers our lives, and ORNL researchers are deeply involved in every aspect of the electricity ecosystem, including improved batteries and battery charging (see "Going wireless for better vehicle charging," page 14). ORNL research also runs the gamut from basic research on new materials (see "Helping to ensure the supply of critical materials," page 10) to applied research focused on the deployment of new and improved technologies (see "New center houses ORNL electricity research," page 16).

Batteries for electric vehicles, or EVs, are central to transportation research because they have the potential to wean us away from gasoline and diesel fuel, which are responsible for the emission of more than 2 billion tons of carbon dioxide annually in the United States alone.

To realize their potential, however, batteries will have to get better. They will have to charge faster, last longer on a charge and be both safer and cheaper — a key goal, given that the cost of a battery makes up roughly 30 percent of an EV's price tag.

Pursuing solid electrolytes

One important focus of battery research is the electrolyte, the ion-conducting medium between anode and cathode. Traditionally, the electrolyte has been a liquid, which limits both the safety and stability of a battery.

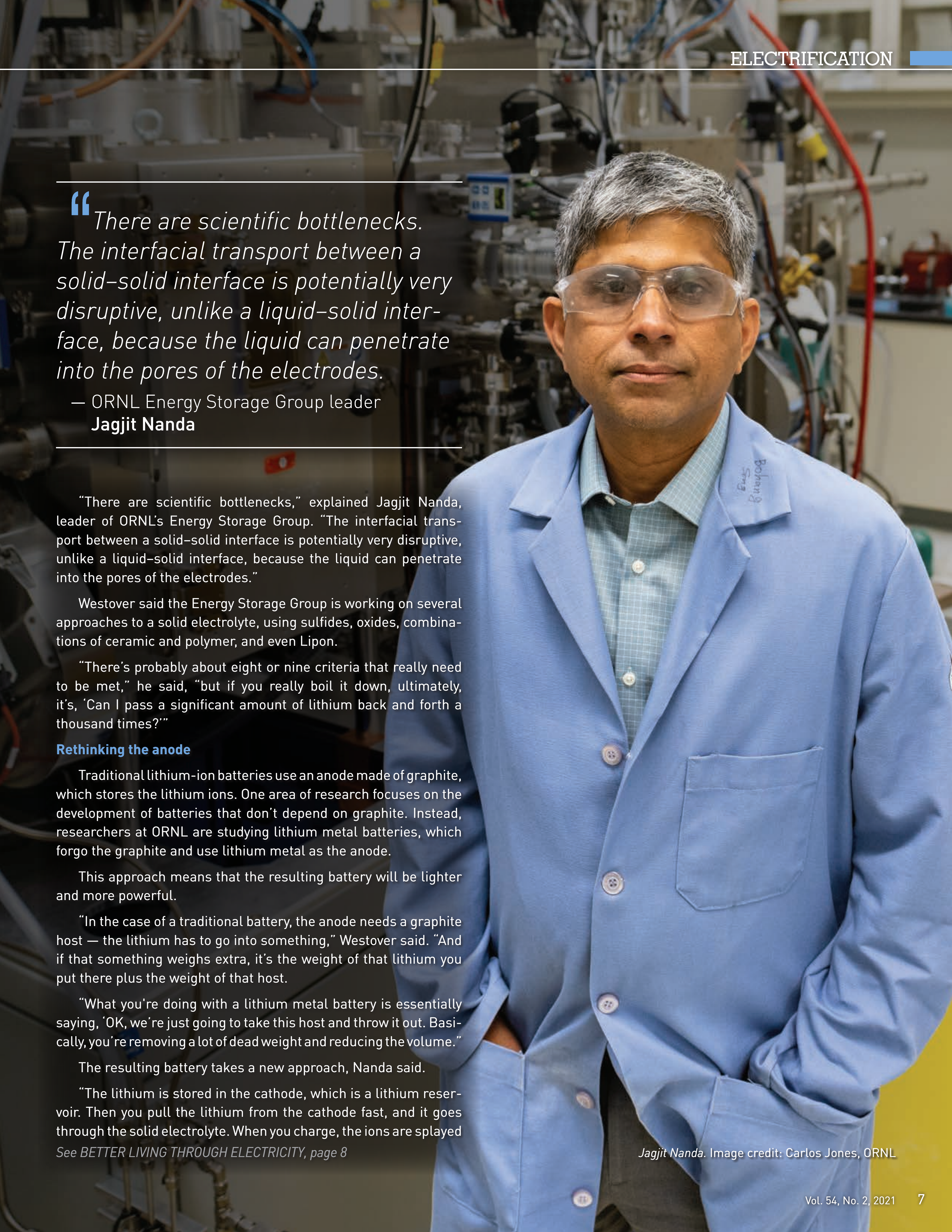
Much of the problem is that liquid electrolytes are flammable. When things go wrong — say a battery is damaged or overheats — it can burst into flames.

"The reason your phone might catch fire is there's a flammable solution in your battery," said ORNL materials scientist Andrew Westover. "If you set a match to it, it'll burn like gasoline."

ORNL researchers are addressing this shortcoming by developing solid electrolytes, which do not burst into flame.

The lab has a long history working with solid electrolytes. In 1991, for example, ORNL researchers developed a solid electrolyte called Lipon, which enabled thin-film batteries for applications such as "hazard cards," which alerted the wearer to the presence of hazardous gases in the environment.

Making modern batteries with a solid electrolyte, however — ones able to power EVs for 300 miles or more — is a mammoth undertaking. One challenge is to get an adequate connection between the electrolyte and the anode and cathode.



> *"There are scientific bottlenecks. The interfacial transport between a solid–solid interface is potentially very disruptive, unlike a liquid–solid interface, because the liquid can penetrate into the pores of the electrodes.*
> — ORNL Energy Storage Group leader
> **Jagjit Nanda**

"There are scientific bottlenecks," explained Jagjit Nanda, leader of ORNL's Energy Storage Group. "The interfacial transport between a solid–solid interface is potentially very disruptive, unlike a liquid–solid interface, because the liquid can penetrate into the pores of the electrodes."

Westover said the Energy Storage Group is working on several approaches to a solid electrolyte, using sulfides, oxides, combinations of ceramic and polymer, and even Lipon.

"There's probably about eight or nine criteria that really need to be met," he said, "but if you really boil it down, ultimately, it's, 'Can I pass a significant amount of lithium back and forth a thousand times?'"

Rethinking the anode

Traditional lithium-ion batteries use an anode made of graphite, which stores the lithium ions. One area of research focuses on the development of batteries that don't depend on graphite. Instead, researchers at ORNL are studying lithium metal batteries, which forgo the graphite and use lithium metal as the anode.

This approach means that the resulting battery will be lighter and more powerful.

"In the case of a traditional battery, the anode needs a graphite host — the lithium has to go into something," Westover said. "And if that something weighs extra, it's the weight of that lithium you put there plus the weight of that host.

"What you're doing with a lithium metal battery is essentially saying, 'OK, we're just going to take this host and throw it out. Basically, you're removing a lot of dead weight and reducing the volume."

The resulting battery takes a new approach, Nanda said.

"The lithium is stored in the cathode, which is a lithium reservoir. Then you pull the lithium from the cathode fast, and it goes through the solid electrolyte. When you charge, the ions are splayed

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Jagjit Nanda. Image credit: Carlos Jones, ORNL

BETTER LIVING THROUGH ELECTRICITY, page 7

on a current collector. And when you discharge, the battery does the work, and the lithium is restored to the cathode efficiently."

If this approach is successful, the energy density of the resulting battery will nearly double, from 250 to up to 500 watt-hours per kilogram, according to Westover.

"Essentially, that means if you had the same weight of battery, it would last twice as long without needing to charge," he said.

The challenges to this approach include longevity — typically, these batteries can't go through nearly as many charging cycles — and the creation of lithium formations called dendrites.

"When you plate lithium metal without a host to contain it," Westover said, "oftentimes what happens is you form something called lithium dendrites — long lithium needles that will pierce the electrolyte and cause a short between your anode and your cathode."

This is especially bad news if you have a liquid electrolyte, which is subject to fire.

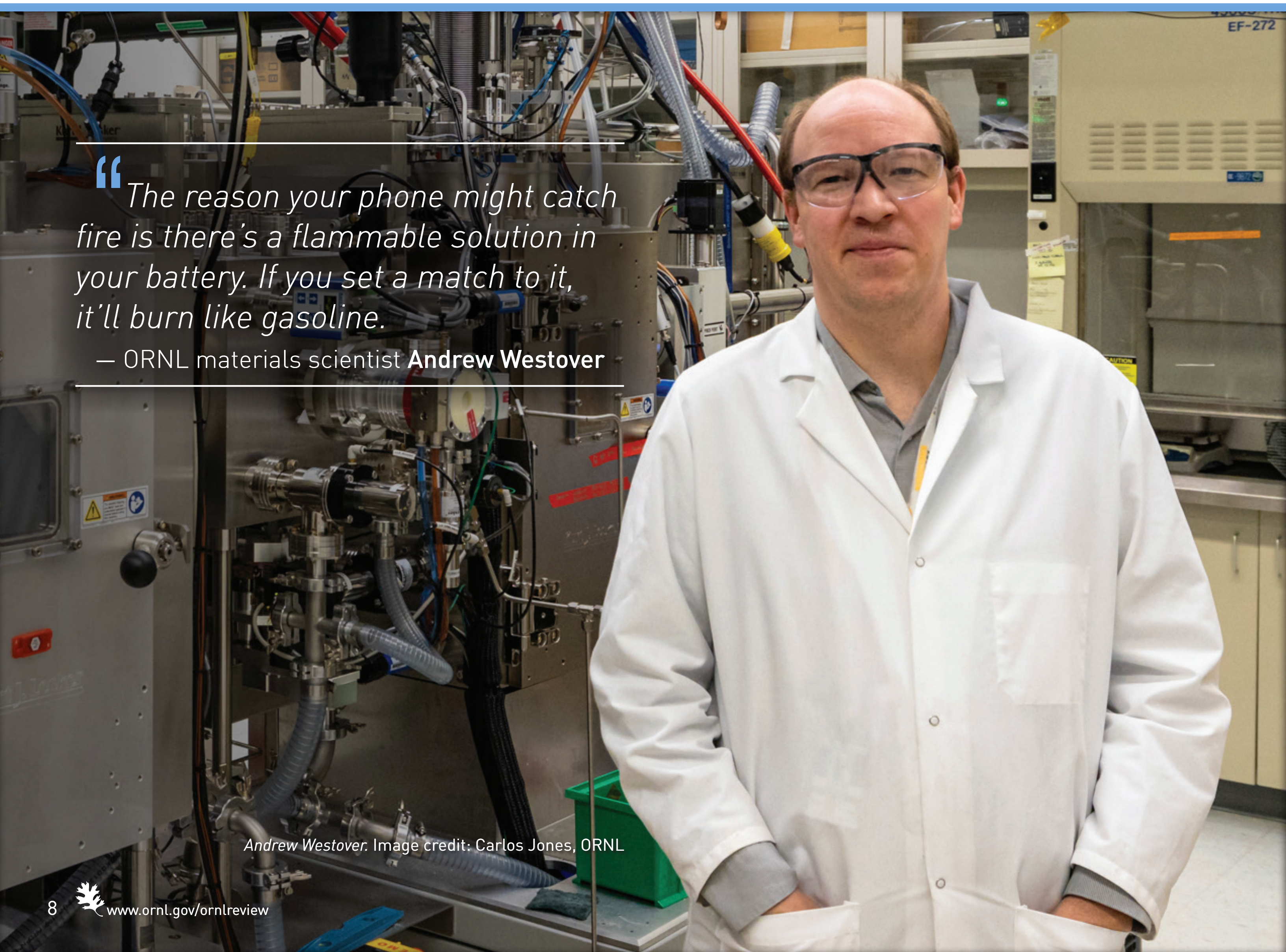
How these issues will be resolved remains to be determined, Westover said.

"It's pretty easy to say we use a lithium metal, but there's actually a lot of questions," he said. "Do we need a little bit of lithium there to get us started, like a seed layer? How much do impurities affect performance? And then, really importantly, how does the interface with the lithium metal shape and form?"

Cobalt-free cathodes

Another focus of ORNL research is development of a battery cathode that doesn't use cobalt, a metal that is both expensive and prone to supply issues.

Cobalt — in the form of lithium cobalt oxide — has been critical to the success of lithium-ion batteries since they were developed in the 1990s, according to Ilias Belharouak, head of the lab's Electrification Section. In particular, he said, cobalt is critical to the stability and performance of the battery.



> *"The reason your phone might catch fire is there's a flammable solution in your battery. If you set a match to it, it'll burn like gasoline.*
> — ORNL materials scientist **Andrew Westover**

Andrew Westover. Image credit: Carlos Jones, ORNL

"The question is, are we going to get the same performance as we do with today's lithium-ion batteries? You cannot have people, instead of utilizing their phone for a whole day, having to recharge many times a day. People enjoy certain standards, and you have to at least meet those standards.
— ORNL Electrification Section Head
Ilias Belharouak

Ilias Belharouak. Image credit: Carlos Jones, ORNL

Unfortunately, we're not going to have enough cobalt to go around, and supply bottlenecks may be especially troublesome for North America, which has relatively little cobalt.

"Cobalt is not sustainable," Belharouak said. "Why? Because we don't have a lot of it in the U.S. If you take the U.S. and Canada, they only produce about 4 percent of the worldwide supply."

For years, companies have worked to reduce the amount of cobalt in lithium-ion batteries. Tesla is using a substitute, called NCA, that is 80 percent nickel, 15 percent cobalt and 5 percent aluminum. According to Belharouak, that's the least cobalt we have in a commercial car battery so far, but it's not good enough.

"Even with that 15 percent, the cobalt needs if we were to scale these technologies to, let's say, millions of EVs, will be massive."

In response, Belharouak's group has developed a cobalt-free cathode using a material known as NFA, which is a mixture of nickel, iron and aluminum. The new material promises to deliver the same stability and all the benefits of cobalt — including fast charging, cost effectiveness and long lifetimes — while cutting costs. In addition, the NFA cathodes will be able to use the same manufacturing infrastructure as cobalt-based cathodes.

These benefits — especially strong performance — are critical for any cathode material that can replace cobalt, Belharouak said. In essence, the new materials must be as good as the old ones.

"The question is, are we going to get the same performance as we do with today's lithium-ion batteries? You cannot have people, instead of utilizing their phone for a whole day, having to recharge many times a day. People enjoy certain standards, and you have to at least meet those standards."

An electric future

This ORNL research supports a vehicle industry that is moving rapidly toward EVs and away from the internal combustion engine. The United Kingdom, for instance, plans to phase out new gasoline- and diesel-powered vehicles by 2030, and General Motors has announced plans to go all-electric by 2035.

"I think the battle for electric vehicles has pretty much been won," Westover said. "It's just a matter of time until it dominates the market."

Organic chemist Santa Jansone-Popova works on developing solvents that efficiently extract rare-earth minerals from the ore that contains them — and from one another. Image credit: Carlos Jones, ORNL

Ensuring the supply of critical materials

by Jim Pearce
pearcejw@ornl.gov

Our society's ability to transition to clean energy technologies depends, to a great extent, on having adequate supplies of the materials needed to manufacture components that will be ubiquitous in a clean energy economy — particularly batteries and electric motors.

Diversifying supply

One way that ORNL helps to ensure adequate supplies of these materials is through its participation in the Critical Materials Institute, one of DOE's Energy Innovation Hubs, led by Ames Laboratory. ORNL Corporate Fellow Bruce Moyer, who heads CMI's Diversifying Supply Focus Area, noted that the laboratory has made significant advances in this field.

Among these critical materials are rare-earth metals, a group of 17 elements used in technological applications such as magnets. Unfortunately, their concentrations in nature don't match our demand for them.

"In the most common ore, just two rare earths account for 75 percent of the amount of rare earths present, cerium and lanthanum," Moyer said. "The rare earth that we need the most is neodymium, and it makes up about 15 percent. So we have to mine five times as much cerium and lanthanum to supply the neodymium that we need for magnets."

One solution to this imbalance is to find new uses for these overabundant metals, increasing both their value and the profitability of mining them.

ORNL Distinguished research scientist Ramesh Bhave developed the Membrane Solvent Extraction technology, which can be used to recover lithium, cobalt, manganese and nickel from recycled lithium-ion batteries. Image credit: Carlos Jones, ORNL

"So we came up with the idea to look for unique uses for cerium in aluminum alloys," Moyer explained. "This was an idea that former ORNL staff scientist Orlando Rios brought to us with a partner from ECK Industries."

They proposed developing a new aluminum–cerium alloy for transportation applications, which last year consumed over 1 million metric tons of aluminum in the United States. Meeting part of that demand with an aluminum–cerium alloy could significantly increase demand for cerium.

"A strong demand for cerium means that rare-earth mines producing neodymium could increase their revenue streams by hundreds of millions of dollars per year," Moyer said. "That would increase their profitability and competitiveness."

ECK wanted to know whether this alloy is castable, so CMI funded a project to research this question. Rios's team, with ECK as partner, found that the alloy would be as castable as the best aluminum alloys on the market *and* that some formulations didn't need any heat treatment at all.

"If you can avoid heat treatment, you can cast a part and use it almost as it comes out of the mold," Moyer said.

> "*In the most common ore, just two rare earths account for 75 percent of the amount of rare earths present, cerium and lanthanum. The rare earth that we need the most is neodymium, and it makes up about 15 percent. So we have to mine five times as much cerium and lanthanum to supply the neodymium that we need for magnets.*
>
> — **Bruce Moyer**, head of Critical Materials Institute Diversifying Supply Focus Area

The new alloy proved useful to Emrgy Inc., which specializes in small-scale hydroelectric power for municipalities and agricultural irrigation. The company found that the alloy worked well in hydroelectric turbine blades and began putting the new blades in the field within about three years.

"I've never seen an example of where something has been turned around so fast from an early-stage research idea to a product produced by industry," Moyer said.

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ENSURE THE SUPPLY OF CRITICAL MATERIALS, page 11

Mining motors and batteries

ORNL senior research scientist Tim McIntyre heads the laboratory's rare-earth recovery and reuse efforts, specializing in deconstructing discarded consumer products to retrieve the critical materials they contain. Recent projects have included harvesting magnets from computer hard drives and electric motors as well as extracting critical materials from electric vehicle batteries.

"In the case of hard drives, we're recovering nickel-plated neodymium-iron-boron magnets," McIntyre said. "Thanks to the nickel coating, these magnets are usually in pristine condition and are easy to remove. We're also chasing magnets in larger electric motors, but since these magnets don't have a protective coating, it's more challenging to remove them intact. As a result, we end up with powders and chunks of magnet material."

Material retrieved by these processes can be crushed and remanufactured for new magnet applications.

"We take this material and dissolve it in an acid solution, and whatever is not dissolved is filtered out. That leaves primarily lithium, cobalt, manganese and nickel. Then we use our Membrane Solvent Extraction — or MSX — technology, which first selectively extracts each of these elements. Then, on the other side of the module, each element is back-extracted into another dilute solution of acid or other suitable media. From there, the materials are recovered."

All of the elements are recovered, and the process produces recycled materials that are more than 99.9% pure — pure enough to be used to produce new batteries.

"This turns end-of-life scrap material into materials that can be used again in the battery manufacturing process," Bhave said. "Also, the process is scalable. These membrane modules can be arranged to handle 1,000 tons per year of production capacity."

ORNL has licensed MSX technology and other similar separation technologies to Momentum Technologies, Inc., so the company can explore its potential for recovering critical materials from batteries, magnets and other devices.

"In the case of hard drives, we're recovering nickel-plated neodymium-iron-boron magnets. Thanks to the nickel coating, these magnets are usually in pristine condition and are easy to remove. We're also chasing magnets in larger electric motors, but since these magnets don't have a protective coating, it's more challenging to remove them intact. As a result, we end up with powders and chunks of magnet material.

— ORNL senior research scientist **Tim McIntyre**

"When we recycle electric vehicle batteries, we break them down to individual cathodes, anodes and separation membranes," McIntyre said. "That's where we find the lithium, nickel, cobalt and manganese — key materials for lithium-ion battery production."

McIntyre said a big challenge in making recycling cost-effective is the logistics of processing recycled materials in large quantities. As a result, his team focused on developing high-throughput technology. Despite variations in battery construction from manufacturer to manufacturer, McIntyre and his team successfully demonstrated an automation capable of processing 10 million hard drives per year.

The Li-ion battery processing facility at ORNL's National Transportation Research Center recovers battery cathodes and ships them to industrial partners that extract the lithium, cobalt, nickel and manganese for use in new batteries.

Recovering battery materials from electronic waste

ORNL is also exploring novel ways to increase the recovery of critical materials from e-waste. Ramesh Bhave, ORNL distinguished research scientist and project leader for membrane-based battery materials and rare-earth elements separations, noted that sometimes recycled battery material isn't thoroughly separated.

"You end up getting material that contains everything — cathodes, anodes and other elements from the battery," Bhave said.

Direct conversion: helping to close the recycling gap

Ilias Belharouak is an ORNL distinguished scientist and head of the Electrification and Energy Infrastructure section of the laboratory's Energy and Transportation Sciences Division. He's also deeply involved in developing practical ways to recycle lithium-ion batteries — like those that are used in electric vehicles.

Traditional gas-powered vehicles use lead-acid batteries, 90 percent of which are recycled. That figure is a goal of sorts for Belharouak.

"Compare that 90 percent to the figure for lithium-ion battery recycling," Belharouak said, "which is in the 5 to 10 percent range. That is a huge gap, and it will take years to close it. The issue truly is technology. The technology to recycle materials from lithium-ion batteries efficiently, cost-effectively and in an environmentally friendly manner does not currently exist."

Belharouak noted that this situation poses a growing challenge for battery manufacturers' supply chains.

"If you have an electric vehicle," he said, "after about 10 years, you will have a battery that contains more than 200 kilograms of material that is ready to be recycled. If you don't have the technology to recycle batteries, that creates a supply chain issue. To keep making batteries for EVs, battery manufacturers need to have access to streams of raw materials — minerals and other materials. However, if you have the technology to recycle lithium-ion batteries, that takes some of the pressure off supply chains.

"At a high level, that's what lithium-ion battery recycling is all about."

The third way

Currently, the state of the art for lithium-ion battery recycling consists of two main processes: pyrometallurgical and hydrometallurgical. The pyrometallurgical process involves burning lithium-ion cells and then using chemistry to separate the desirable elements from the resulting slag. The hydrometallurgical process focuses on chemically dissolving batteries and then separating specific elements from the resulting solution.

"Our process provides a third way," Belharouak said. "It's what we call direct recycling. Unlike the other recycling processes, we're recovering the components of the batteries without reducing them to their individual elements."

The direct recycling effort is headquartered at the ReCell Advanced Battery Recycling Center at Argonne National Laboratory. ReCell is a collaboration among Argonne, the National Renewable Energy Laboratory, ORNL, Michigan Technological University, the University of California San Diego, and Worcester Polytechnic Institute. The center's goal is to develop cost-effective, flexible processes for recycling lithium-ion batteries.

The logic behind direct recycling is that, since the battery manufacturer has already paid to process battery materials from scratch, it makes sense to develop a way to recycle battery components without having to process the materials again.

Part of making recycling cost-effective is developing the ability to process end-of-life products in large quantities. Here, a custom gripper is used to lift a lithium-ion battery module. These modules can weigh up to 100 pounds. Image credit: Jonathan Harter, ORNL

For example, one aspect of direct recycling involves using uses triethyl phosphate, a "green" solvent, to separate battery cathodes from metal foil current collectors. These and other recovered components can be reused in new batteries. Currently the direct recycling process recovers battery anodes, cathodes, separators, electrolytes and related hardware.

"This saves both time and money," Belharouak said, "and it delivers benefits in terms of environmental costs as well.

"At the national laboratories, we do the R&D to develop effective processes, and then we scale-up those processes to the point where our industrial partners can take them to the next level. The ReCell center has industrial partners who bring this sort of expertise from all points along the battery supply chain.

"That sort of collaborative R&D is the way to gain ground in this field. Recycling lithium-ion batteries is an R&D problem, and R&D is going to find the solution."

Going wireless for better vehicle charging

by Stephanie Seay
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To make electric vehicle charging even easier than filling up a car with gas, ORNL researchers have demonstrated a range of wireless charging solutions for stationary vehicles and are nearing completion of a new system to charge EVs while they're in motion.

Electrifying transportation is at the top of the list for solutions to decarbonize the American economy. The transportation sector is the largest source of greenhouse gases in the nation, with cars and light trucks alone accounting for 60 percent of emissions. DOE has supported a range of research to make EV ownership more convenient and less costly for consumers, including the goal of a charge time of 15 minutes or less.

With custom magnetic coils, silicon carbide-based power electronics, novel controls and shielding technology to handle stray emissions, ORNL scientists have proven they can wirelessly charge both a light-duty passenger car across a six-inch airgap and a medium-duty delivery truck across an 11-inch airgap at the 20-kilowatt level at greater than 92 percent power transfer efficiency — on par with a wired system. They can even flow power in both directions, enabling vehicles to serve as energy storage.

The researchers have successfully demonstrated a 120 kW wireless charging system with 97 percent efficiency and are planning to install higher voltage systems, up to 270 kW, on passenger vehicles to meet or exceed the 15-minute charging goal.

The systems are built and evaluated at the National Transportation Research Center at ORNL, the only DOE-designated user facility focused on performing early-stage research and development in transportation technologies. The medium-duty vehicle wireless charging demonstration was held at the new Grid Research Integration and Deployment Center — or GRID-C — at ORNL, which combines multiple electrification research across the vehicle, buildings and grid space under one roof.

The researchers now have a finish line in sight for a system called dynamic wireless charging, in which vehicles are automatically energized while rolling over specially equipped roadways. The researchers will make use of a new, one-of-a-kind test bed at GRID-C to evaluate the dynamic wireless charging system and to support research on how the technology will smoothly integrate into the nation's power grid.

The ORNL polyphase magnetic coil has the highest surface power density in the world, making possible a small, lightweight system that can charge electric vehicles in as little as 10 minutes. Image credit: Carlos Jones, ORNL

"Once you get to these higher power levels to enable fast charging, you especially don't want people handling the heavy cables typically required," said Burak Ozpineci, who heads ORNL's Vehicle and Mobility Systems Research Section. "With wireless technology, you wouldn't have to remember to plug in your vehicle at home, and it's always topped off. You just park it in the garage, and it's done. The same with charging pads at workplaces or at extreme-fast wireless charging stations.

"Now we want to take it a step further. What if you have an EV and never have to worry about having enough of a charge to go anywhere you like? We can accomplish that with dynamic wireless charging."

With dynamic charging, for instance, some highway lanes or even on- and off-ramps would be embedded with charging pads, and your car would be charged as you drive it over the coils.

Dynamic charging can also reduce the grid impact resulting from the peak demand of overnight charging in homes or at charging stations, Ozpineci said. Instead, that demand for EV charging would be levelized and allow for better grid stability.

ORNL's dynamic charging goal is a 200 kW system that can quickly charge vehicles at highway speeds. The economics look good. Installing dynamic charging on heavily traveled roadways means the cost of the system would be spread across many users, bringing the cost of ownership down.

Convenient charging could even encourage the adoption of electrified semitrailers, said Veda Galigekere, who leads the Electric Drives Research Group at ORNL. Once the dynamic system undergoes full evaluation at GRID-C, it will be tested at the American Center for Mobility in Michigan.

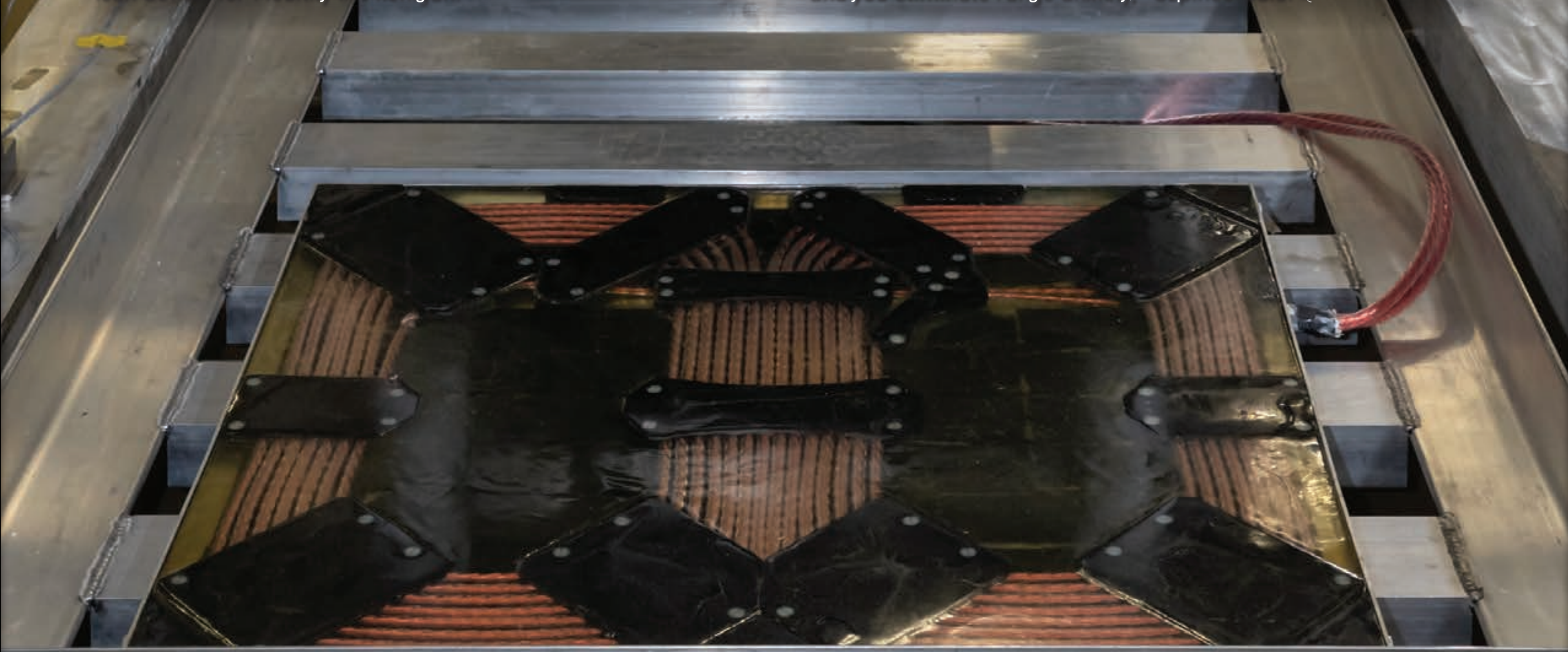
The success of ORNL's wireless charging technology relies heavily on researchers' broad expertise in power electronics, control systems, electrical engineering and electromagnetics. A key development in the evolution of the ORNL wireless tech was the creation of a polyphase magnetic coil coupling design that allows for much higher power density in smaller coils. The design encompasses a three-phase system that features rotating magnetic fields between layers of coils.

Even at the 300 kW level, the ORNL coil design has a much smaller footprint than does currently available wireless charging technology due to that higher surface power density. The ground-based coil is about the size of an extra-large pizza, while the coil on the car is about the size of a small or medium pizza, said Omer Onar, who leads the lab's Vehicle Power Electronics Research Group.

Another important challenge in the work is resolving the issue of stray electromagnetic emissions around the coils. ORNL is developing advanced shielding technology to control those emissions and the heat they can produce. The solution uses nanocrystalline materials together with aluminum to create a magnetic–metallic hybrid shielding technology that dampens emissions. The technology has been validated up to the 50 kW level already, Onar said.

Automatic charging of vehicles resolves a major stumbling block for consumers who are hesitant to buy an EV. While consumers are increasingly aware that the newest EVs offer a lot of power, they also worry about whether they can get where they're going with currently available charging infrastructure.

"If you can charge wirelessly at home, at work, and even when you're on the way, you never have to think about charging your car, and you eliminate range anxiety," Ozpineci said.



ORNL researchers have developed a test bed to help develop technologies to charge electric vehicles as they are driven over specially equipped roadways. Image credit: Carlos Jones, ORNL

New center houses ORNL electricity research

by Leo Williams
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The Grid Research Integration and Deployment Center, or GRID-C, is a 52,000-square-foot facility located in Hardin Valley, about eight miles from ORNL's main campus.

It pulls together ORNL's work in electricity, from ensuring the safety and stability of America's electric grid, to doing the same for neighborhood-wide microgrids, to developing future battery technologies that will enable battery-powered cars and trucks and, eventually, battery-powered aircraft. The center takes advantage of ORNL's world-class expertise in power electronics, creating new devices from concept to deployment across grid, energy storage, mobility and buildings applications.

"A lot of the work within the lab's grid modernization R&D program is being pulled under one roof," explained Tom King, who manages ORNL's sustainable electricity program. "Geography makes a big difference in where people are located. If you're looking at integration of a system of systems, being able to do that under one roof is imperative."

GRID-C has dedicated areas for a dozen research and development areas related to the power grid and electric vehicles. These include:

- Cybersecurity research into secure, resilient grid communications architectures

ORNL researcher Radha Sree Krishna Moorthy programs and test the controller of a Smart Universal Power Electronics Regulator at GRID-C.
Image credit: Carlos Jones

Roll-to-roll calendering machine and roll-to-roll UV curing equipment in the Battery Testing Laboratory at GRID-C. Image credit: Carlos Jones, ORNL

- A Grid Operations Analytics Laboratory that simulates control room operation and incorporates cybersecurity and physical security, sensors, modeling and data analytics
- Grid simulation, including controls hardware, software platform integration and large-scale system emulation and protection
- Advanced sensors research
- Critical materials recovery and reuse
- Distribution-scale grid research, including power electronics and energy storage
- Vehicle systems and electric drivetrain evaluation
- A Battery Manufacturing Facility that will provide open access to areas from materials synthesis to prototyping of vehicle and grid-level battery systems
- A residential-scale grid to emulate homes and neighborhoods and test grid interaction
- Vehicle-to-grid charging and systems integration, which will explore extreme-fast wired and wireless vehicle charging
- High-voltage research
- Advanced component development

"Everything ties to the grid: buildings, vehicles, chargers, everything," said Power Electronics Systems Integration Group Leader Madhu Chinthavali. "To understand how they interact, we need a facility where we can emulate them and put our developments to the test."

As an example, Chinthavali pointed to a fast charger his group is developing using advanced components that are not commercially available. The availability of charging systems at 120, 240 and 480 volts is critical to judging these components.

"We want to test them, evaluate them and show how different they are," he said, "in terms of efficiency, functionality, and size, weight and volume. For that I need a lab to test it."

Chinthavali also stressed GRID-C's value as a place where industry collaborators can tap into both the experimental equipment and the expertise of ORNL staff in battery technology and grid research.

"Say I'm a hardware vendor who has an extreme fast charger," he said. "We can bring those vendors into this facility, they can tie to the ecosystem, understand the grid interaction with it."

These resources are especially important for business startups that have great ideas but little money, Chinthavalli stressed. ORNL has various funding mechanisms for giving these businesses access to facilities and equipment they could not afford on their own. As such, ORNL is helping them through the "valley of death" between prototypes and commercial-scale technologies.

"This should be a system where we help the startups to cross the 'valley of death,'" he said. "To put up hardware systems like this takes millions and millions of dollars. If they have an idea, they should be able to incubate with us and transform their technology enough to show mass production out of this building."

King agreed that GRID-C opens up opportunities for collaboration, pointing to ORNL's work with Chattanooga, Tennessee's Electric Power Board on small neighborhood-sized grids called microgrids.

"Company partners like EPB will want to make sure that the approaches we're taking aren't going to have major negative impacts in the field," he said. "And so if we work through the technical challenges within GRID-C, hopefully, it'll be ready for field deployment."

Getting ready for an exascale supercomputer

by Coury Turczyn
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When ORNL's new exascale supercomputer, Frontier, completes installation later this year, it will debut as a landmark in high-performance computing, with groundbreaking performance of greater than 1.5 exaflops, or 1.5 quintillion calculations per second. But right now — before Frontier's technological advances are made available to the world's scientists — the room it will occupy is undergoing a complete mechanical, electrical and structural transformation.

Frontier will reside in the former data center of the lab's Titan. Once the most powerful supercomputer in the world, Titan was decommissioned in 2019 after seven years of service. It took about a month for a team of HPE Cray technicians to dismantle 430,000 pounds worth of Titan components and remove them for recycling. Just days later, work began to revamp the 20,000-square-foot room to accommodate Frontier's much higher requirements for power, cooling and structural support. That meant everything had to be stripped out: piping, electrical infrastructure, even the floor.

Workers prepare for ORNL's Frontier supercomputer.
Image credit: Carlos Jones, ORNL

"Titan at peak probably consumed about 10 megawatts of power. At peak, Frontier will consume about 30 megawatts," said Justin Whitt, program director for the Oak Ridge Leadership Computing Facility. "If you use more power, you have to get rid of additional heat, so we are adding the equivalent of 40 megawatts of cooling capacity, about 11,000 tons of refrigeration, for Frontier — much bigger pipes to distribute cool water to the computer."

With demolition completed, a team of about 100 contractors and ORNL craft employees has been installing that new infrastructure, welding in serpentine piping both above and below the huge, empty room while simultaneously building out a new raised floor. Now completed, the floor consists of over 4,500 tiles weighing 48 pounds each — or more than 100 tons altogether.

Long before the data center's construction began — even before the demolition work to gut the room — another massive building project had to be tackled: a mechanical room for all the machinery that will feed cooling water to Frontier. The new supercomputer's cooling water towers will have a system volume of 130,000 gallons, with four 350-horsepower pumps that can each move over 5,000 gallons per minute of the high-temperature water through the Frontier system. The pumps will connect to the data center via 500 feet of 24-inch pipe.

Planners had to find a big enough area for all this infrastructure, as there was no space left in the actual data center. They ended up going to the building next door, and, although it could provide the needed space, it also had some architectural hurdles.

"The building that we're putting the mechanical plant into was originally designed as a lab space, with not a lot of structure to it — it was basically just holding up the roof," said Bart Hammontree, technical project manager for ORNL's Laboratory Modernization Division. "But we're putting in the neighborhood of a million pounds' worth of piping and cooling towers on the roof of this building. So we had to basically build a new structure inside of an existing building, and we had to put new foundations in to support all that."

A construction project of this scale normally takes about two years to complete, Whitt said, but to put Frontier into service as soon as possible, the team plans to complete the work in less than a year and a half.

"The biggest challenge that we face at this point is just the incredibly aggressive schedule that we set for the work," Whitt said. "We're responding to the science need for exascale computers, so we had to accelerate the time frame for everything — for the technologies, for having the room ready. We're doing more work for the OLCF than we've ever done before, and we're doing it on a shorter time scale."

Summit boosts resolution of weather simulation

by Coury Turczyn
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Using ORNL's Summit supercomputer, a team of researchers from the European Centre for Medium-Range Weather Forecasts, or ECMWF, and ORNL have achieved a computational first: a global simulation of the Earth's atmosphere at a 1-square-kilometer average grid-spacing for a full four-month season.

> "In this project, we have now shown for the first time that simulations at this resolution can be sustained over a long time span — a full season — and that the large amount of data that are produced can be handled on a supercomputer such as Summit. We provide factual numbers for what it takes to realize these simulations, and what one may expect both in terms of data volumes and scientific results. We therefore provide a baseline against which future research may be evaluated.
>
> — **Nils Wedi**, head of Earth System Modelling at the European Centre for Medium-Range Weather Forecasts

Completed last June, the milestone marks a big improvement in resolution for the Integrated Forecasting System, also known as the "European Model," which currently operates at 9-kilometer grid-spacing for routine weather forecast operations. It also serves as the first step in an effort to create multiseason atmospheric simulations at high resolution, pointing toward the future of weather forecasting — one powered by exascale supercomputers capable of a billion billion calculations each second.

"In this project, we have now shown for the first time that simulations at this resolution can be sustained over a long time span — a full season — and that the large amount of data that are produced can be handled on a supercomputer such as Summit," said Nils Wedi, head of Earth System Modelling at ECMWF. "We provide factual numbers for what it takes to realize these simulations, and what one may expect both in terms of data volumes and scientific results. We therefore provide a baseline against which future research may be evaluated."

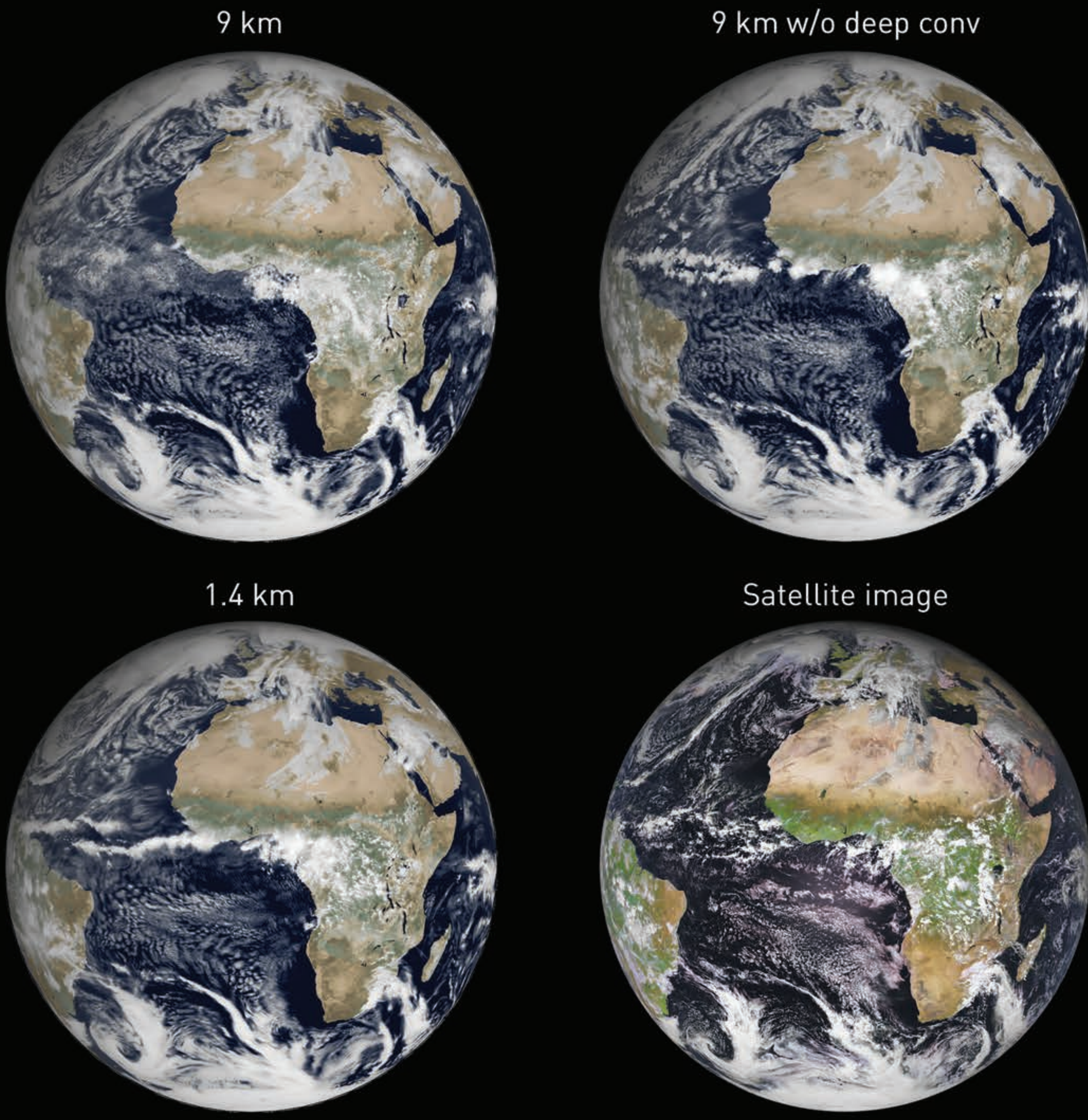
Established in 1975, the ECMWF is an intergovernmental organization composed of 34 member and cooperating countries, providing numerical weather predictions to its members while also selling forecast data to commercial weather services. The original IFS code was written some 30 years ago and has been one of the leading global weather forecast systems in the world, continually updated and optimized for use on many generations of supercomputers at ECMWF. However, to advance their code's performance and scalability, ECMWF researchers also tested it on other high-performance computing systems including Summit, the United States' fastest supercomputer for open science housed at the Oak Ridge Leadership Computing Facility, and the decommissioned Titan.

Armed with compute time from the DOE's Innovative and Novel Computational Impact on Theory and Experiment program, Wedi and his team aim to deliver a "quantum leap" forward in simulating and understanding the Earth's weather and climate.

With the higher resolution of 1-kilometer grid-spacing, the team's simulations are able to represent variations in topography with finer detail. This increased detail results in better airflow characteristics that help determine global circulation patterns.

What's more, the 1-kilometer grid-spacing also enables the representation of processes in the atmosphere that were previously too small to be accounted for with the 9-kilometer grid-spacing. Now, tropical thunderstorms — which move warm, moist air into the upper atmosphere in a process called deep convection — can be simulated explicitly in the models, providing a better look at tropical atmospheric motions.

"We are not simply looking at whether we can make an improvement at any given locality, but ideally all these things should translate into a global circulation system," said Val Anantharaj, an ORNL computational scientist who serves as data liaison



These simulated satellite images of the Earth show the improved resolution of the ECMWF Integrated Forecasting System from 9-kilometer grid-spacing with parametrized deep convection (top left), 9-kilometer grid-spacing without parametrized deep convection (top right), and the 1-kilometer grid-spacing (bottom left). On the bottom right is a Meteosat Second Generation satellite image at the same verifying time. Image courtesy ECMWF/EUMETSAT.

on the project. "If we can resolve the global atmospheric circulation pattern better, then we should be able to produce better forecasts."

Anantharaj said the project's long-term goal is to simulate the remaining seasons to yield a model for one full year. Currently, the team is running another four months of simulations to cover an Atlantic hurricane season. Such high-resolution models can provide virtual laboratories that further our understanding of how the climate is evolving and how weather may look in a future climate.

These simulations can also be used to predict the impact of future high-resolution models employed on exascale platforms such as ORNL's upcoming Frontier system.

"The handling and data challenges that we have overcome during this project are still very large, and our simulations are at the edge of what is achievable today," Wedi said. "However, I believe that it will be possible to run simulations with 1-kilometer grid-spacing routinely in the future — in the same way we are running simulations with 9-kilometer grid-spacing today. To continue to push these boundaries is important."

Supercomputers help explain DNA proofreading

by Rachel McDowell
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DNA replication is one of the most important processes in biology, responsible for ensuring that a cell's genetic material is copied over to new cells efficiently during cell division. But what happens when there is a mistake?

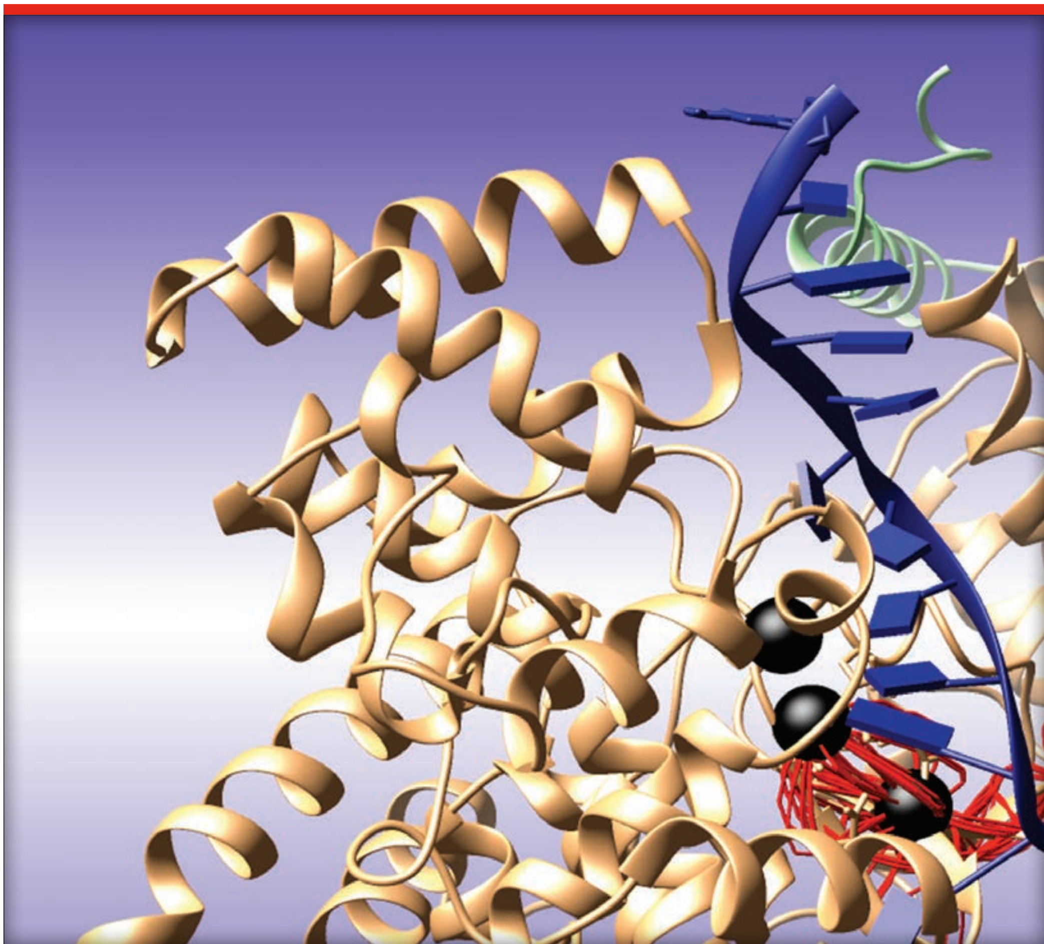
Fortunately, replicative DNA polymerases — the cell's replication molecular machines — are capable of proofreading the newly synthesized DNA and correcting mistakes made during the DNA replication process. These polymerases detect misincorporated DNA bases and transfer them to a specialized compartment inside of the polymerase to excise them.

If it weren't for these versatile and efficient machines, the cell's genetic material would be compromised, potentially leading to abnormal cellular functioning, impaired development and diseases such as cancer. But just how mistakes are corrected while the polymerase synthesizes a new DNA strand hasn't been fully understood.

A team at Georgia State University recently used the Summit supercomputer at ORNL to find the optimal transition path that a highly accurate bacterial DNA polymerase uses to switch between building and editing DNA. This optimal DNA path serves as a molecular highway, guiding the starting point of the DNA strand as it travels the large distance between the two sites where DNA is synthesized or excised. The work was published in *Nature Communications.*

"We represented the path between these two — the polymerase and exonuclease states — as a series of replicas of the simulation system that were all optimized and sampled simultaneously," said Ivaylo Ivanov, a researcher at Georgia State University. "Only with recent advances in GPU technology on massively parallel computing platforms like Summit did it become possible for us to sample the conformational ensemble along the optimal path."

Because all classes of DNA polymerases have a separation between the polymerase and exonuclease states, the team's discovery of a defined pathway linking the two active sites suggests that a path between these states is a universal feature of high-fidelity DNA replication, which is essential for safeguarding the integrity of the genome.



Multitasking at the molecular scale

During DNA replication, enzymes called DNA polymerases read existing DNA strands to create new ones, adding DNA building blocks called nucleosides to single strands to create new double-stranded molecules.

> "We represented the path between these two — the polymerase and exonuclease states — as a series of replicas of the simulation system that were all optimized and sampled simultaneously. Only with recent advances in GPU technology on massively parallel computing platforms like Summit did it become possible for us to sample the conformational ensemble along the optimal path.
>
> — Georgia State University researcher Ivaylo Ivanov

High-fidelity DNA polymerases are remarkably precise, introducing a mistake on average only once in a million DNA base incorporations.

"Yet, when you take this in the context of the entire genome, replication could still result in an astronomical number of errors if no correction happens," Ivanov said.

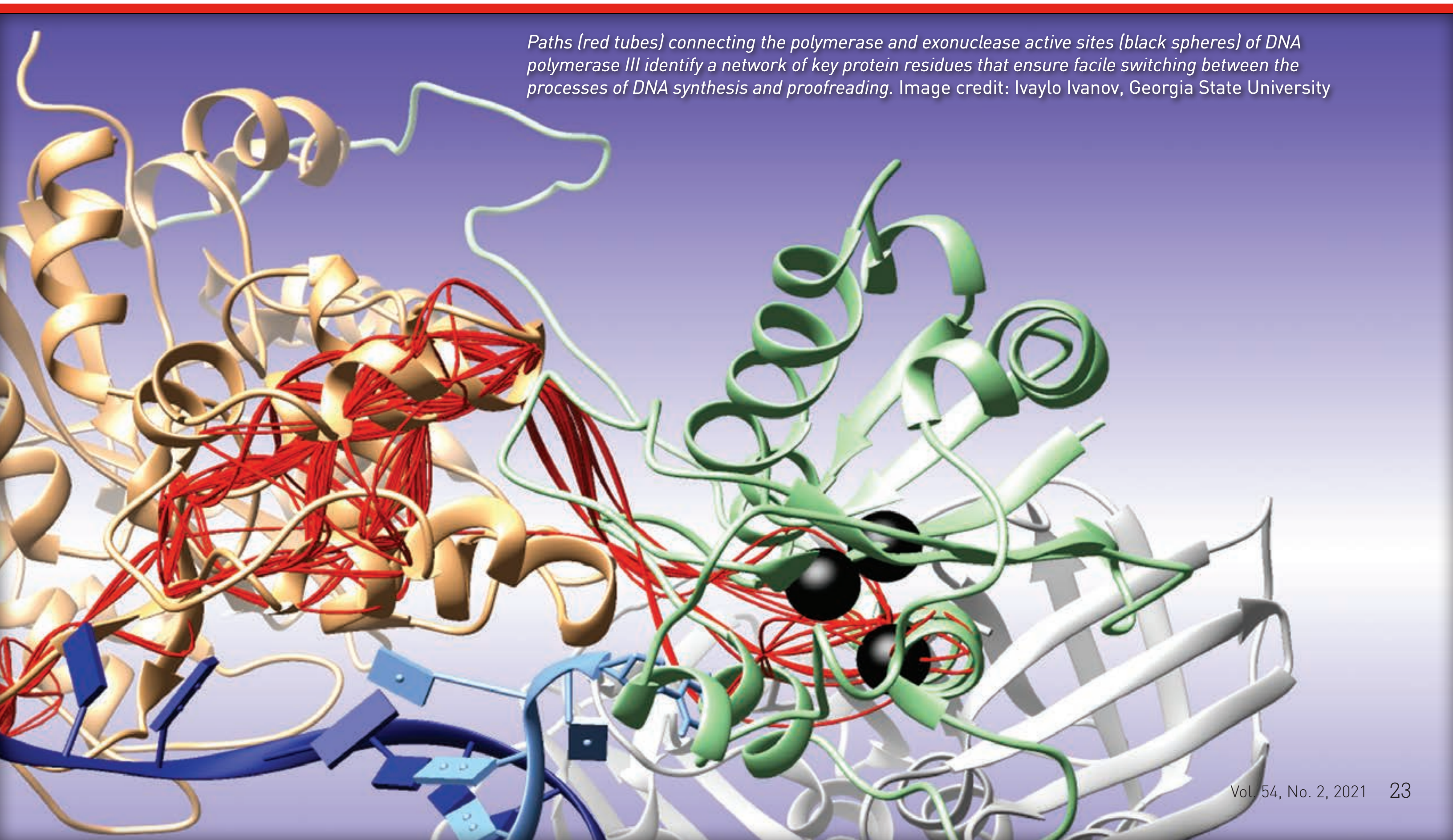
Luckily, DNA polymerases can identify and correct these rare errors. One such replication machine with a built-in error correction mechanism is DNA polymerase III, or Pol III, from the *E. coli* bacteria. Scientists have known that Pol III can switch between its DNA-building and DNA-editing tasks rapidly, but they haven't known how it transitions from one state to the other.

Using the Nanoscale Molecular Dynamics code combined with novel data analysis methods, Ivanov's team modeled the optimal path for switching between Pol III's synthesizing and editing states. The computational results were successfully validated in biochemical experiments performed by a research group headed by Professor Meindert Lamers from Leiden University Medical Center in the Netherlands.

The researchers also analyzed the intermediate stages along the path and gained the ability to provide realistic timescales directly comparable to biochemical experiments.

Insights gleaned from studies such as these hold promise for applications in biotechnology and biomedicine. Understanding how bacterial polymerases function could help scientists counter bacterial infections, for example.

The team plans to extend the Pol III study to other DNA polymerases and continue exploring this important mechanism. Additionally, the path optimization approach adopted in this study could prove invaluable in modeling structural transitions in other complex biological systems in the future.



Paths (red tubes) connecting the polymerase and exonuclease active sites (black spheres) of DNA polymerase III identify a network of key protein residues that ensure facile switching between the processes of DNA synthesis and proofreading. Image credit: Ivaylo Ivanov, Georgia State University

Physicists

improve precision of neutrino studies

by Dawn Levy
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A new study led by ORNL will improve researchers' ability to characterize unwanted background signals in specialized neutrino detectors. As a result, experiments should be better able to detect real signals from these weakly interacting, electrically neutral subatomic particles, elucidating their role in the universe.

"We've identified a reaction with significant discrepancies between our new measurement and the historical data," said ORNL physicist Michael Febbraro, who led the study, which presents an improved measurement of the reaction.

One older measurement from 2005, which had been used as a reference standard, considered only the ground state of particles, rather than a spectrum of ground and excited states. The new measurement, taken using a detector array based on neutron spectroscopy and secondary gamma rays, considered the entire spectrum of particle energies.

Febbraro, who conceived the experiment and built the detectors, performed the measurement with physicists Richard deBoer of the University of Notre Dame and Steven Pain of ORNL.

A well-known nuclear reaction — the carbon-13 alpha-n reaction — is a major contributor to background in experiments that measure neutrinos, whether they are emitted from the sun, atmosphere, accelerators, nuclear reactors or the Earth's core.

The rate of that reaction needs to be well known to accurately calculate background in detectors such as Japan's Kamioka liquid scintillator antineutrino detector, or KamLAND. Using a University of Notre Dame accelerator, the researchers shot an alpha particle — a helium-4 nucleus — at a target of carbon-13, briefly forming oxygen-17, which decayed into oxygen-16 and a neutron. The researchers measured the probability of that background-creating reaction, which is proportional to the rate of neutron production, taking place inside the detector while it's looking for neutrino signals.

"We found that the current world data set is incorrect by quite a bit, because they didn't account for other reaction channels that turn on," Febbraro said. "We have a special type of detector which can tell what the neutron energy is, and that was the main enabling technology which made this measurement possible."

> *"We've identified a reaction with significant discrepancies between our new measurement and the historical data.*
>
> — ORNL physicist **Michael Febbraro**

Neutrino detectors need to be big to boost weak signals. KamLAND is filled with a hydrocarbon-based scintillator, an oil that interacts with neutrinos and emits light. Those sparkles make it easier to spot and count elusive neutrinos. However, the decay products of radon, a naturally occurring radioactive gas, combine with carbon-13, a rare isotope present in the scintillator, creating oxygen-16 and neutrons that mimic signals from neutrinos.

KamLAND weighs approximately a thousand tons. So, while carbon-13 accounts for only 1.1% of all carbon, KamLAND contains 11 tons of it. Radon entering the detector decays into daughter elements having different energies. The alpha particles produced by those decays interact with carbon-13, creating a background that overwhelms the neutrino signal.

"Background is something that you have to precisely understand," said ORNL physicist Kelly Chipps, who helped to analyze the data and interpret the results with ORNL physicist Michael Smith. "Otherwise, the number of real events that you saw might be completely wrong."

Chipps said asking a large, scintillator-filled neutrino detector to distinguish background from signal is like being blindfolded, fed chocolates with either a red or green candy coating, and asked to tell how many red chocolates you ate.

"Trouble is, all the candies taste the same," said Chipps. "To figure out how many red candies you ate, you'd count the total number of candies and call the chocolate manufacturer to ask how many red candies are generally in a bag."

Just as knowing this ratio would let you estimate candy quantities, the reference information in evaluated nuclear databases lets scientists estimate neutrino numbers.

The new neutron production rate that Febbraro and his colleagues found can now be used by physicists working on KamLAND and other liquid scintillator–based neutrino experiments to subtract background with better accuracy and precision.

Since presenting this new measurement, Febbraro's team has employed the detector to measure similar reactions. They have found discrepancies in neutron production rates for half a dozen isotopes. "Calculations in this mass region are not very reliable," he said.

For more information: https://go.usa.gov/xAF48

At the University of Notre Dame, part of the Oak Ridge Deuterated Spectroscopic Array measured a reaction that causes noise in some neutrino detectors.
Image credit: Michael Febbraro, ORNL

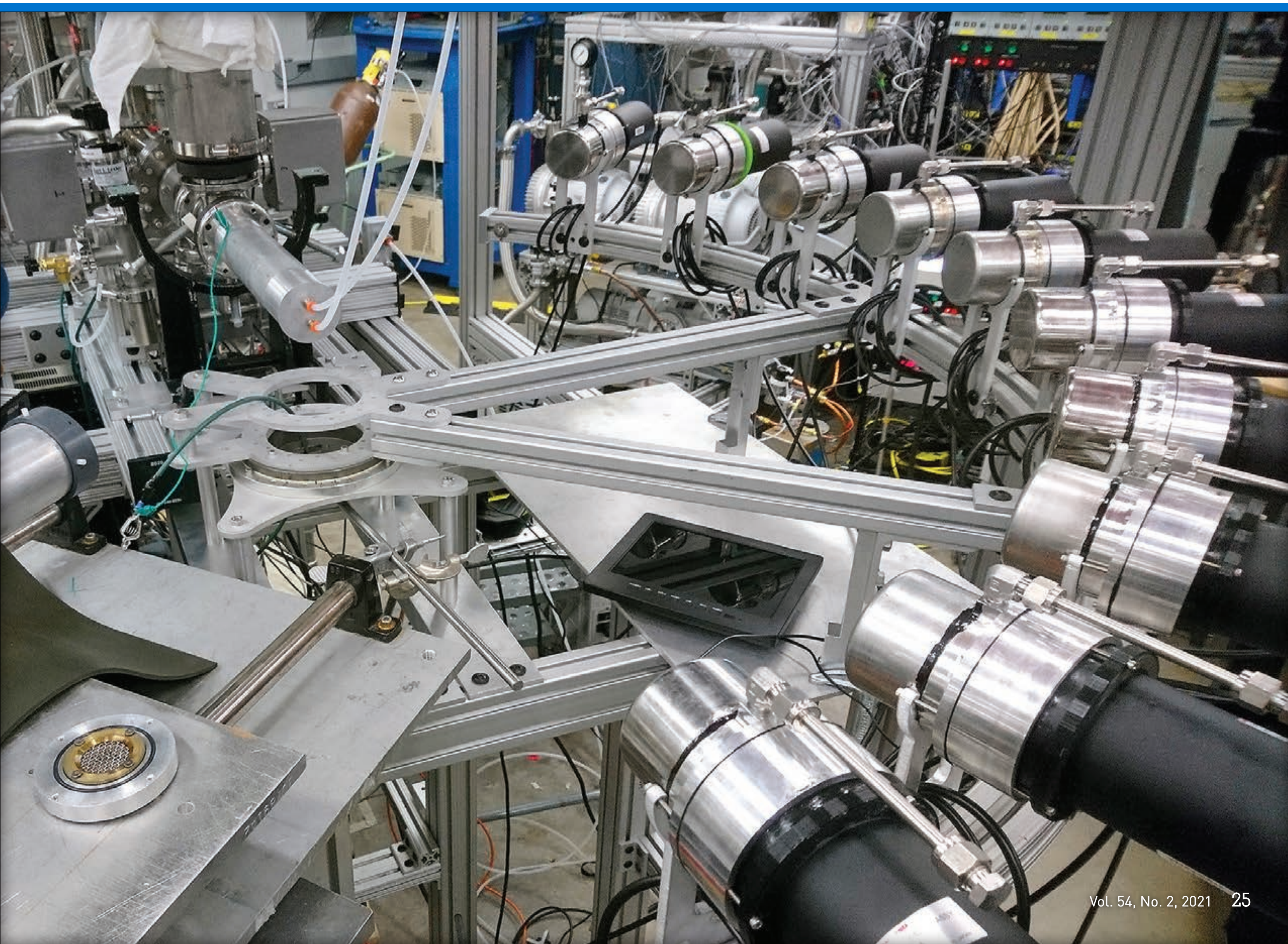

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Image credit: Nathan Armistead and Adam, Malin, ORNL

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New technique improves next-gen solar cells

by Dawn Levy
levyd@ornl.gov

Led by ORNL and the University of Tennessee, Knoxville, a study of a solar-energy material with a bright future revealed a way to slow phonons, the waves that transport heat. The discovery could improve novel hot-carrier solar cells, which convert sunlight to electricity more efficiently than conventional solar cells by harnessing photogenerated charge carriers before they lose energy to heat.

"We showed that the thermal transport and charge-carrier cooling time can be manipulated by changing the mass of hydrogen atoms in a photovoltaic material," said ORNL's Michael Manley. "This route for extending the lifetime of charge carriers reveals new strategies for achieving record solar-to-electric conversion efficiency in novel hot-carrier solar cells."

When sunlight strikes a solar cell, photons create charge carriers — electrons and holes — in an absorber material. Hot-carrier solar cells quickly convert the energy of the charge carriers to electricity before it is lost as waste heat. Preventing heat loss is a grand challenge for these solar cells, which have the potential to be twice as efficient as conventional solar cells.

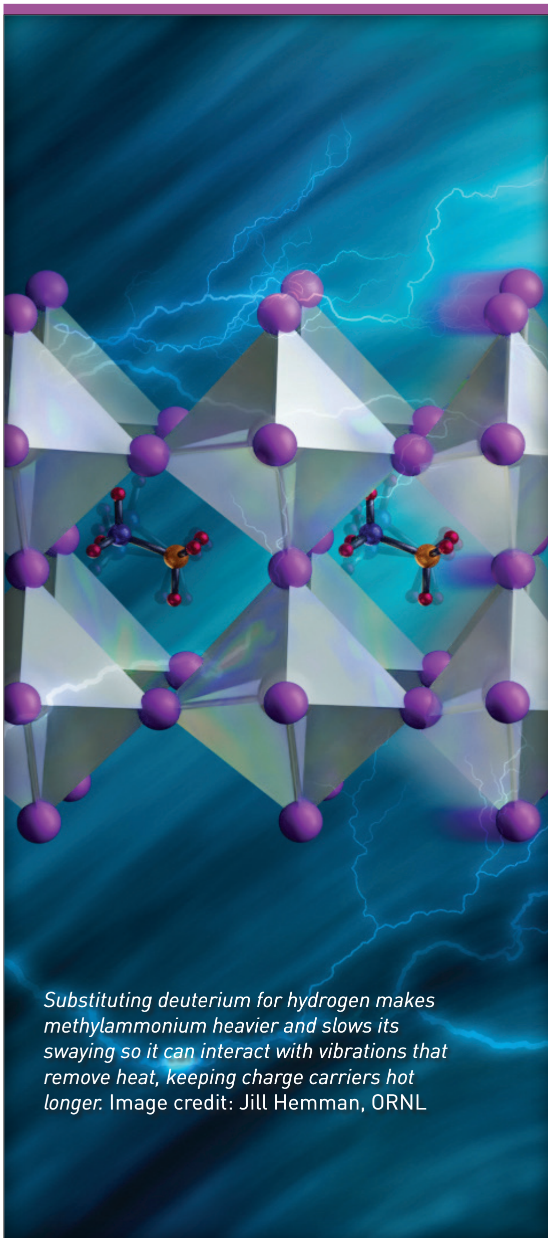
The conversion efficiency of conventional perovskite solar cells has improved from 3 percent in 2009 to more than 25 percent in 2020. A well-designed hot-carrier device could achieve a theoretical conversion efficiency approaching 66 percent.

The researchers studied methylammonium lead iodide, a perovskite absorber material. In its lattice, collective excitations of atoms create vibrations. Vibrations moving in sync with each other are acoustic phonons, whereas those moving out of sync are optical phonons.

"Typically, charge carriers first lose their heat to optical phonons, which propagate slower than acoustic phonons," explained ORNL co-author Raphael Hermann. "Later, optical phonons interact with acoustic phonons that carry away this energy."

However, in a region called the hot phonon bottleneck, exotic physics prevents electrons from losing their energy to collective vibrations that transport heat. To enhance this effect in a photovoltaic perovskite, the researchers used inertia, the tendency of an object to keep doing what it's doing, be that resting or moving.

"We basically slowed down how fast the molecules can sway, similar to slowing



Substituting deuterium for hydrogen makes methylammonium heavier and slows its swaying so it can interact with vibrations that remove heat, keeping charge carriers hot longer. Image credit: Jill Hemman, ORNL a spinning ice skater by putting weights in her hands," Hermann said.

UT Knoxville's Mahshid Ahmadi and ORNL's Kunlun Hong led the synthesis of methylammonium lead iodide crystals at ORNL's Center for Nanophase Materials Sciences. They substituted a lighter isotope of hydrogen — normally occurring protium, which has no neutrons — with a heavier one — deuterium, which has one neutron — in the perovskite's central methylammonium molecule.

Next, Manley and Hermann, with ORNL's Songxue Chi, mapped phonon dispersion in protonated and deuterated crystals at ORNL's High Flux Isotope Reactor. The lab's Luke Daemen revealed all possible vibrational energies at ORNL's Spallation Neutron Source.

In addition, ORNL's Hsin Wang performed thermal diffusivity measurements at ORNL's High Temperature Materials Laboratory to investigate how heat moved in the crystals. "Those measurements told us that deuteration decreased the already-low thermal conductivity," Manley said.

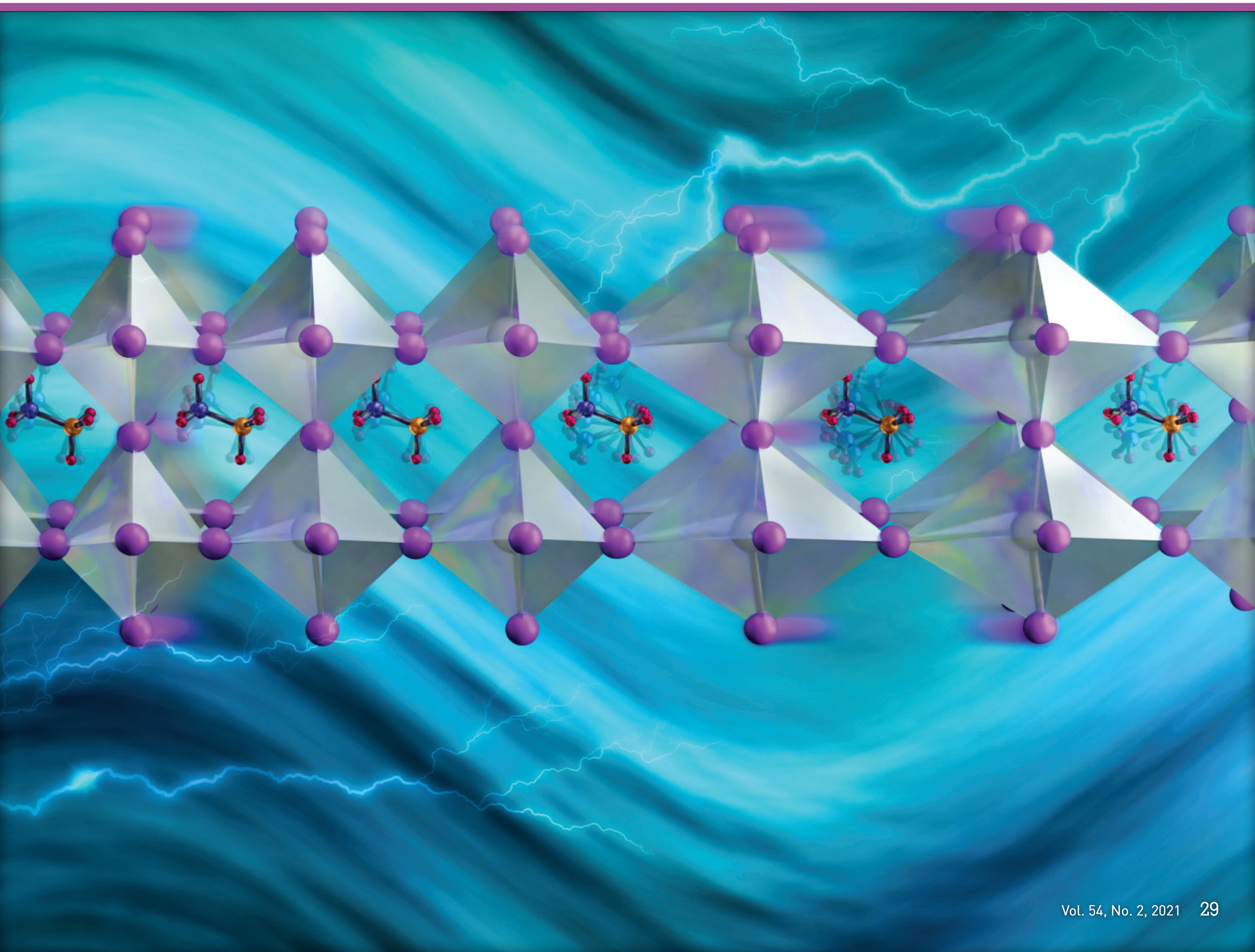
Deuteration slowed heat transport so much that the charge-carrier cooling time was expected to double. ORNL's Chengyun Hua confirmed this finding with pump–probe laser experiments to measure the electrons' energy dissipation in the deuterated and protonated perovskites.

The discovery made in the ORNL–UT Knoxville-led study may provide a bright spot for future manufacturers of hot-carrier solar cells.

"Phonons look like a pretty effective knob to turn, and we know how to turn the knob," Manley said. "When you want to improve the materials, you can modify the molecule that you add, methylammonium or something else. The finding can inform developers' decisions about how they grow their crystals."

Added Ahmadi, "This knowledge can be used to guide materials design for applications beyond photovoltaics, such as optical sensors and communication devices."

For more information: https://go.usa.gov/xAMb6



Quantum light

squeezes the noise out of microscopy signals

by Dawn Levy
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ORNL researchers have used quantum optics to advance state-of-the-art microscopy and illuminate a path to detecting material properties with greater sensitivity than is possible with traditional tools.

"We showed how to use squeezed light — a workhorse of quantum information science — as a practical resource for microscopy," said Ben Lawrie of ORNL's Materials Science and Technology Division, who led the research with Raphael Pooser of ORNL's Computational Sciences and Engineering Division. "We measured the displacement of an atomic force microscope microcantilever with sensitivity better than the standard quantum limit."

Unlike today's classical microscopes, Pooser and Lawrie's quantum microscope requires quantum theory to describe its sensitivity. The nonlinear amplifiers in ORNL's microscope generate a special quantum light source known as squeezed light.

"Imagine a blurry picture," Pooser said. "It's noisy, and some fine details are hidden. Classical, noisy light prevents you from seeing those details. A 'squeezed' version is less blurry and reveals fine details that we couldn't see before because of the noise." He added, "We can use a squeezed light source instead of a laser to reduce the noise in our sensor readout."

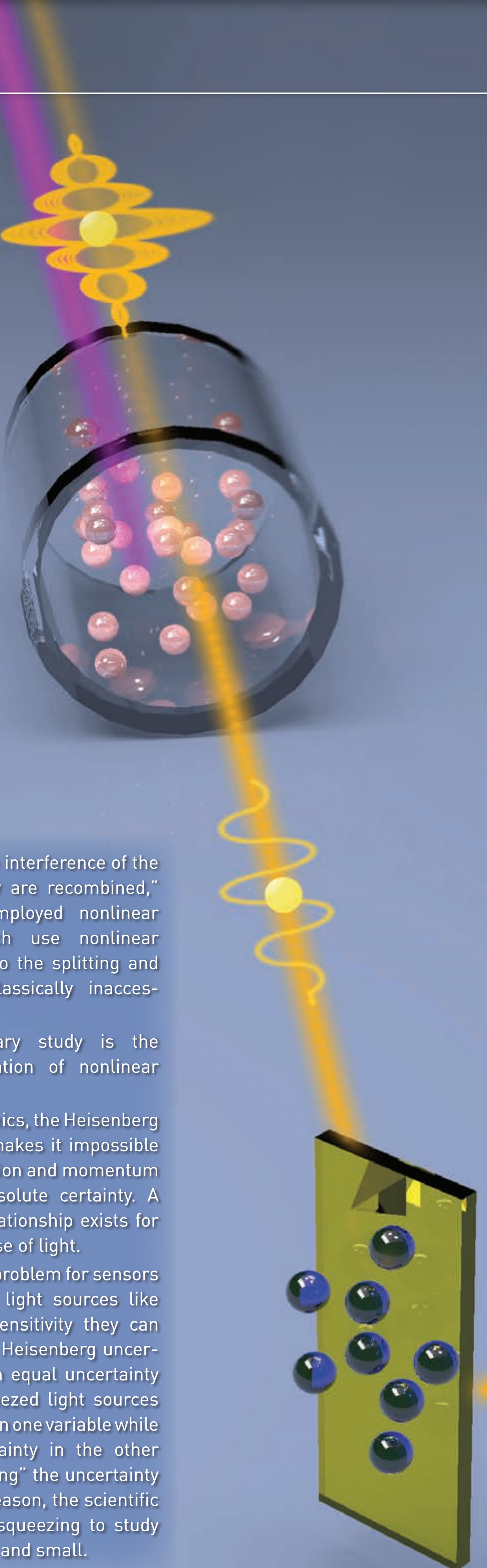
The microcantilever of an atomic force microscope is a miniature diving board that methodically scans a sample and bends when it senses physical changes. With student interns, Lawrie and Pooser showed that the quantum microscope they invented could measure the displacement of a microcantilever with 50% better sensitivity than is classically possible. For one second–long measurements, the quantum-enhanced sensitivity was 1.7 femtometers — about twice the diameter of a carbon nucleus.

"Squeezed light sources have been used to provide quantum-enhanced sensitivity for the detection of gravitational waves generated by black hole mergers," Pooser said. "Our work is helping to translate these quantum sensors from the cosmological scale to the nanoscale."

Their approach to quantum microscopy relies on control of lightwaves. When lightwaves combine, they can interfere constructively (amplitudes of peaks add to make the resulting wave bigger) or destructively (trough amplitudes subtract from peak amplitudes to make the resulting wave smaller). This effect can be seen in waves in a pond or in an electromagnetic wave of light like a laser.

"Interferometers split and then mix two light beams to measure small changes

> *"We showed how to use squeezed light — a workhorse of quantum information science — as a practical resource for microscopy. We measured the displacement of an atomic force microscope microcantilever with sensitivity better than the standard quantum limit.*
>
> — ORNL Materials Science and Technology Division researcher **Ben Lawrie**



in phase that affect the interference of the two beams when they are recombined," Lawrie said. "We employed nonlinear interferometers, which use nonlinear optical amplifiers to do the splitting and mixing to achieve classically inaccessible sensitivity."

The interdisciplinary study is the first practical application of nonlinear interferometry.

In quantum mechanics, the Heisenberg uncertainty principle makes it impossible to define both the position and momentum of a particle with absolute certainty. A similar uncertainty relationship exists for the amplitude and phase of light.

That fact creates a problem for sensors that rely on classical light sources like lasers: The highest sensitivity they can achieve minimizes the Heisenberg uncertainty relationship with equal uncertainty in each variable. Squeezed light sources reduce the uncertainty in one variable while increasing the uncertainty in the other variable, thus "squeezing" the uncertainty distribution. For that reason, the scientific community has used squeezing to study phenomena both great and small.

"In this experiment, we were able to exploit properties of entanglement," Pooser said.

Entanglement occurs when independent objects behave as one. Einstein called it "spooky action at a distance." In this case, the intensities of the light beams are correlated with each other at the quantum level.

"Because of entanglement, if we measure the power of one beam of light, it would allow us to predict the power of the other one without measuring it," Pooser continued. "Because of entanglement, these measurements are less noisy, and that provides us with a higher signal-to-noise ratio."

ORNL's approach to quantum microscopy is broadly relevant to any optimized sensor that conventionally uses lasers for signal readout. "Conventional interferometers could be replaced by nonlinear interferometry to achieve quantum-enhanced sensitivity for biochemical sensing, dark matter detection or the characterization of magnetic properties of materials," Lawrie said.

ORNL researchers developed a squeezed light approach for atomic force microscopy that enables measurement of signals otherwise buried by noise. Squeezed light waves are commonly used in quantum information science research.
Image credit: Raphael Pooser, ORNL

Making mightier 'magnetic motors'

by Paul Boisvert
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Electric motors might be better described as "magnetic" motors.

That's because the electricity supplied to them, typically from a battery or power grid, is used to control a series of magnets — and it's the magnetic forces that do most of the work of producing the motor's power output.

Scientists from GE Research, in collaboration with researchers at ORNL, have developed and used neutron scattering to help characterize a new type of "magnetic" motor. GE's unique design features a relatively soft magnetic steel material capable of having its magnetism controlled at the millimeter scale in virtually any pattern, which permits higher power densities and efficiencies than electric motors made from conventional silicon steel.

By combining ceramic masks and gas nitrogenation — that is, treating the alloy with nitrogen — GE can meet design requirements by controlling the material's level of magnetization from zero to 100 percent at every position, without removing any of the material itself. Nonmagnetic areas can be positioned to provide enhanced mechanical strength for high-speed applications.

"Conventional high-performance electric motors require permanent magnets made of expensive rare-earth materials, plus their rotors are usually made of magnetic laminates that cause energy loss due to the high magnetization in the mechanical supportive locations, thus reducing the desired magnetic interaction between the stator and rotor," said Min Zou, project leader for the GE program.

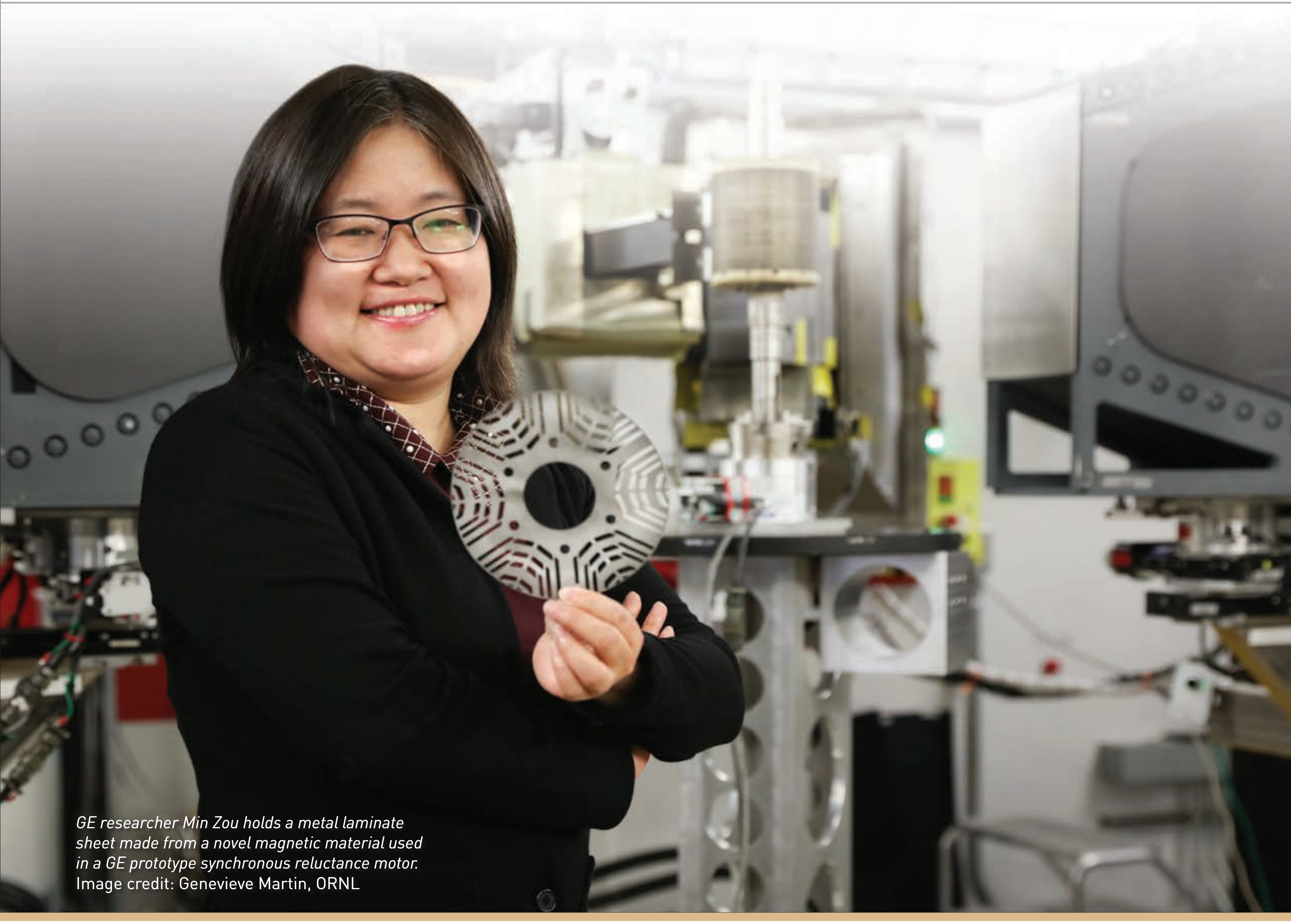
"Our unique synchronous reluctance motor design helps reduce costs by eliminating the use of rare-earth permanent magnets, and our ability to pattern the magnetic and nonmagnetic areas of a rotor optimizes the magnetic circuit, so the rotor can turn more efficiently and with greater power."

The GE prototype rotor consists of a stack of hundreds of individual sheets of the magnetic material, called laminates, which are nitrogenated at high temperature after having a ceramic mask applied to control the spread of nitrogen in the desired pattern. The masked regions remain magnetic, while the exposed regions transform to nonmagnetic. The masks are removed prior to assembling the laminates into the rotor stack.

GE originally approached ORNL's Physical Sciences Directorate for technical assistance in evaluating the effects of the high-heat nitrogenating process on the soft magnetic material.

PSD researchers Craig Bridges, Mike Brady and Orlando Rios, with postdoctoral research associate Hunter Henderson, worked with GE's scientists to develop a processing method

Metal laminate sheet made from a novel magnetic material. Image credit: Genevieve Martin, ORNL



GE researcher Min Zou holds a metal laminate sheet made from a novel magnetic material used in a GE prototype synchronous reluctance motor.
Image credit: Genevieve Martin, ORNL

to produce the magnetic alloy in rolled sheets as thin as one-hundredth of an inch. They also helped create a unique process used to define the areas that have their magnetism turned off, as well as chemical and mechanical methods of removing the masks.

Once the laminate production process was established, GE wanted to examine the prototype laminates for signs of warping and internal residual stress resulting from internal distortions during processing, which could weaken the material. Because part of the magnetic patterns are buried deep inside the stack of metal laminates, neutron scattering was the best solution because of its highly penetrating properties.

> *"We conducted the residual stress analysis experiments at VULCAN, the world's premier neutron instrument for studying phase and residual stress distribution in large industrial samples. Unlike X-rays, neutrons are able to penetrate deeply into metals, and VULCAN was able to produce data on the residual stresses of different phases of the laminates inside the stack.*
>
> — Neutron scattering scientist **Ke An**

"We conducted the residual stress analysis experiments at VULCAN, the world's premier neutron instrument for studying phase and residual stress distribution in large industrial samples," said Ke An, a neutron scattering scientist at the Spallation Neutron Source. "Unlike X-rays, neutrons are able to penetrate deeply into metals, and VULCAN was able to produce data on the residual stresses of different phases of the laminates inside the stack."

The team's experimental results indicate there are significant residual stresses that are not uniformly distributed, which agrees with the stress distribution calculated by GE mechanical engineers. Actual measured residual stress data will help with future laminate designs to reduce warpage and maintain mechanical integrity.

Sulfur-scavenging bacteria affect crops and climate

by Kim Askey
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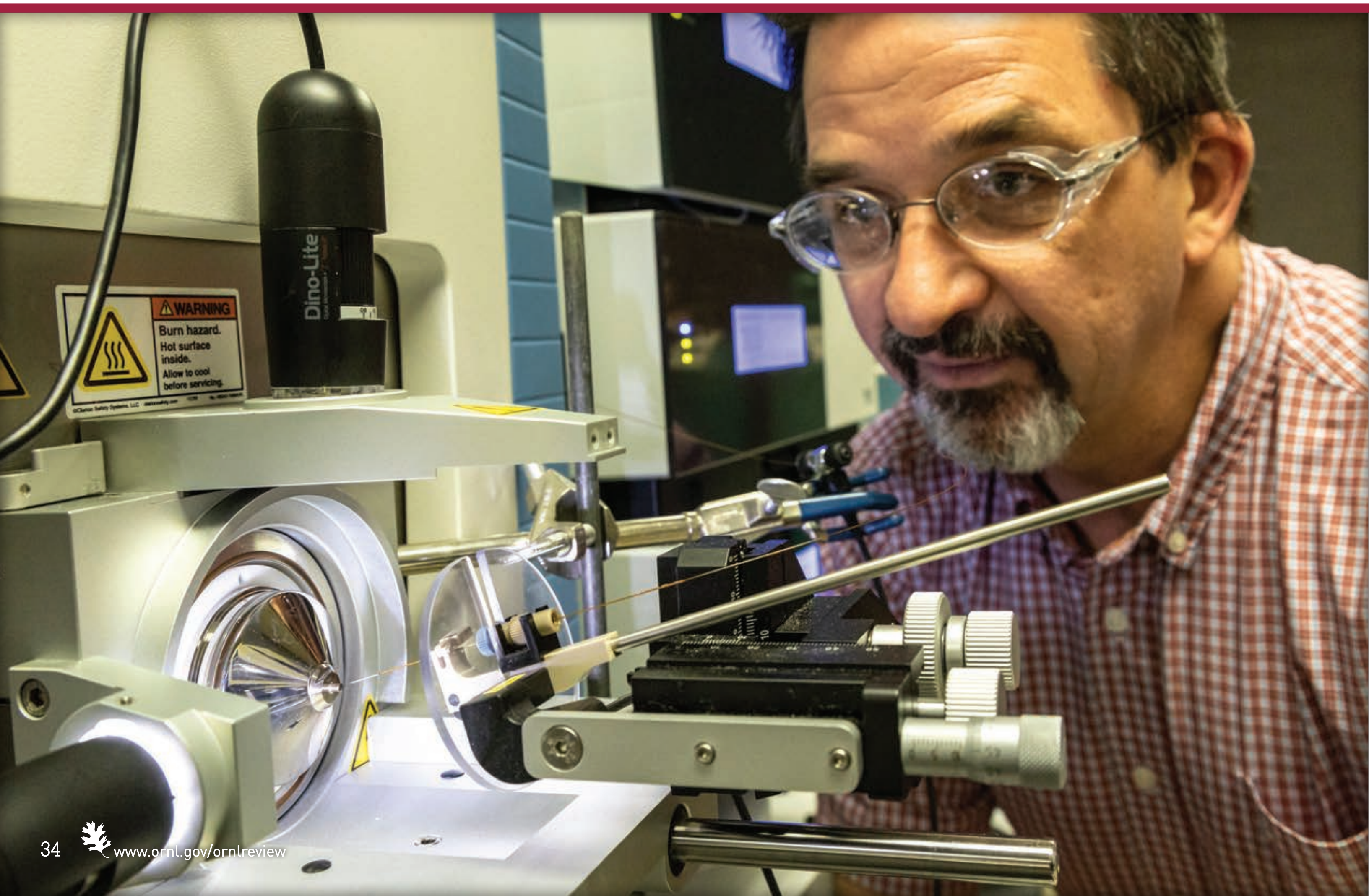
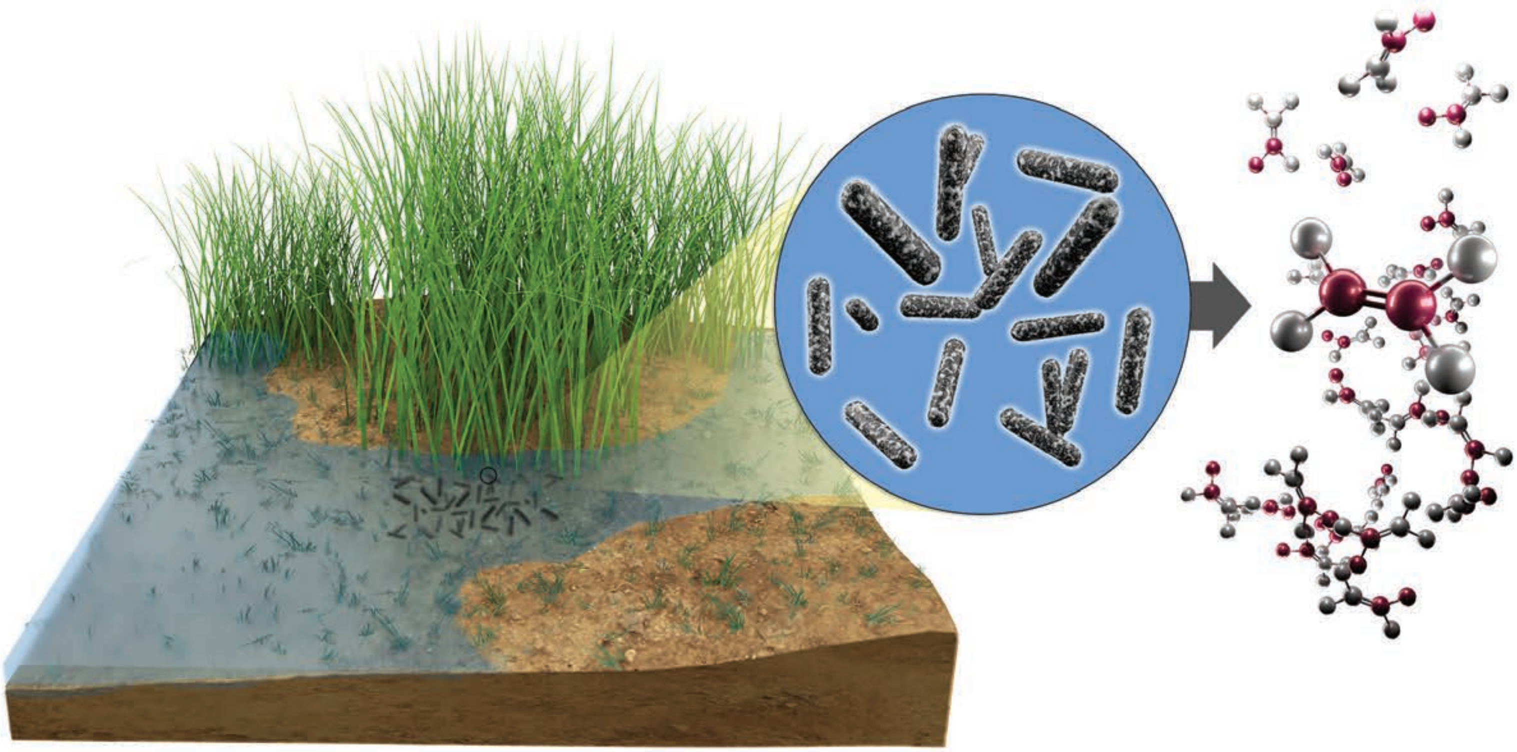
Scientists at ORNL and Ohio State University have discovered a new microbial pathway that produces ethylene, a hormone that regulates growth in plants and can trigger crop damage if overly abundant.

The discovery, published in the journal *Science*, sheds light on a long-standing mystery about how ethylene is produced in waterlogged, oxygen-deprived soils and points to potential treatment methods to prevent crop damage. The study also outlines a previously unknown way bacteria generate methane, a powerful greenhouse gas.

Researchers found that ethylene and methane are byproducts of a bacterial process that makes methionine, an amino acid necessary for building proteins. When their environment is anaerobic and low in sulfur, bacteria are forced to scavenge sulfur from cellular waste products, triggering this new pathway.

ORNL Bioanalytical Mass Spectrometry Group leader Bob Hettich used a specialized mass spectrometry technique to characterize the proteomes of microbial systems. Image credit: Carlos Jones, ORNL





Scientists have discovered how microbes in waterlogged soils produce high levels of ethylene, which can adversely affect agricultural crops and bioenergy feedstocks like switchgrass. Image credit: Andy Sproles, ORNL

The research began at Ohio State, where scientists were studying a completely different topic: carbon fixation in photosynthetic bacteria. One day, OSU researcher Justin North decided to measure the gases being consumed and emitted by *Rhodospirillum rubrum* when these microbes were starved for sulfur. He was surprised to detect ethylene.

"We know these bacteria are producing hydrogen and consuming carbon dioxide," North said. "But, lo and behold, they were making copious amounts of ethylene gas. And we thought, well, that's weird."

North studied this new metabolic process using radioactive compounds to track the production of methionine and ethylene in microbes. But a different type of analytical biotechnology was needed to make the critical link between the pathway and the proteins called enzymes that drive it.

Ohio State reached out to Bob Hettich, who leads the Bioanalytical Mass Spectrometry Group at ORNL, for a comparative analysis of the collection of proteins, called proteomes, present in these bacteria under two different scenarios: low-sulfur, ethylene-producing conditions and high-sulfur, nonethylene-producing conditions.

Hettich's group has developed a cutting-edge approach to characterizing the proteomes of microbial systems using mass spectrometry. He and postdoctoral researcher Weili Xiong identified thousands of proteins from the low- and high-sulfur systems and analyzed their comparative abundances to pinpoint a handful of proteins for further study.

"We found striking differences," Hettich said.

The data showed a family of proteins similar to the enzymes called nitrogenases that convert atmospheric nitrogen to ammonia, a well-studied process that is essential to life on Earth. These nitrogenase-like proteins were almost 50 times more abundant in the ethylene-producing samples. Some iron- and sulfur-related proteins also increased in abundance when sulfur was scarce, pointing to a possible new pathway for sulfur metabolism.

These data were surprising, as nitrogenase-like proteins are grouped in genomic databases with nitrogenases that have similar DNA sequences. Given their name, these nitrogenase-like proteins are not ones the scientists would have guessed play a role in sulfur metabolism.

"Sometimes the naming or annotation of a gene or gene family can be misleading," Hettich said. "The name suggests a primary function. In fact, the gene might have a secondary function, a night job so to speak, or it might actually be doing something completely different."

"But the data are the data," he continued. "If you run the measurements correctly and in an agnostic fashion, where you don't know the answer a priori, then the data will reveal the real connections."

With these crucial data, Ohio State researchers and collaborators ran a series of experiments manipulating the bacterial genome. When they included or removed a specific gene cluster, it turned ethylene production on and off like a switch, confirming the genes are essential to this metabolic pathway. Depending on the source of sulfur used, bacteria produce ethylene or methane as byproducts.

The discovery creates a host of new scientific questions, including several lines of inquiry that may have substantial benefit in preventing ethylene damage to bioenergy and agricultural crops.

Neutrons map COVID-19 replication mechanism

by Jeremy Rumsey
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To better understand how the novel coronavirus behaves and how it can be stopped, scientists have completed a 3D map that reveals the location of every atom in an enzyme molecule critical to SARS-CoV-2 reproduction.

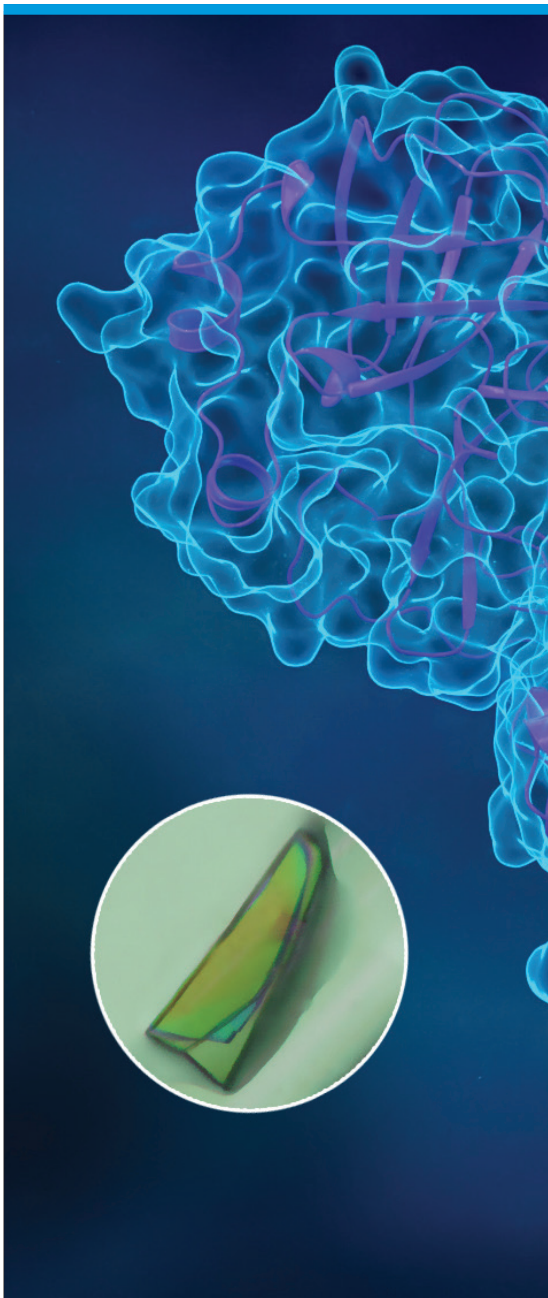
ORNL researchers used neutron scattering to identify key information to improve the effectiveness of drug inhibitors designed to block the virus's replication mechanism. The research was published in *the Journal of Biological Chemistry*.

The SARS-CoV-2 virus, which causes COVID-19, assembles long chains of proteins composed of approximately 1,900 amino acids. For the virus to reproduce, those chains have to be broken down and cut into smaller strands by an enzyme called the main protease. The active protease enzyme is formed from two identical protein molecules held together by hydrogen bonds. Developing a drug that inhibits or blocks protease activity will prevent the virus from replicating and spreading to other cells in the body.

"This new information is exactly what is needed to design inhibitors with a higher degree of specificity, ensuring the inhibitor molecules are binding very tightly to their intended targets and disabling the protease," said co-author Andrey Kovalevsky.

Neutron experiments first revealed that, contrary to previously held beliefs, the site containing the amino acids where the protein chains are cut is in an electrically charged reactive state and not in a resting, or neutral, state. Second, they mapped the location of each hydrogen atom in the places where inhibitors would bind to the protease enzyme, as well as the electrical charges of the associated amino acids. The experiments also charted the entire network of hydrogen bonds between the protein molecules that hold the enzyme together, enabling it to initiate the chemical process of cutting the protein chains.

"Half of the atoms in proteins are hydrogen. Those atoms are key players in enzymatic function and are essential to how drugs bind," Kovalevsky said. "If we don't know where those hydrogens are and how the electrical charges are distributed



inside the protein, we can't design effective inhibitors for the enzyme."

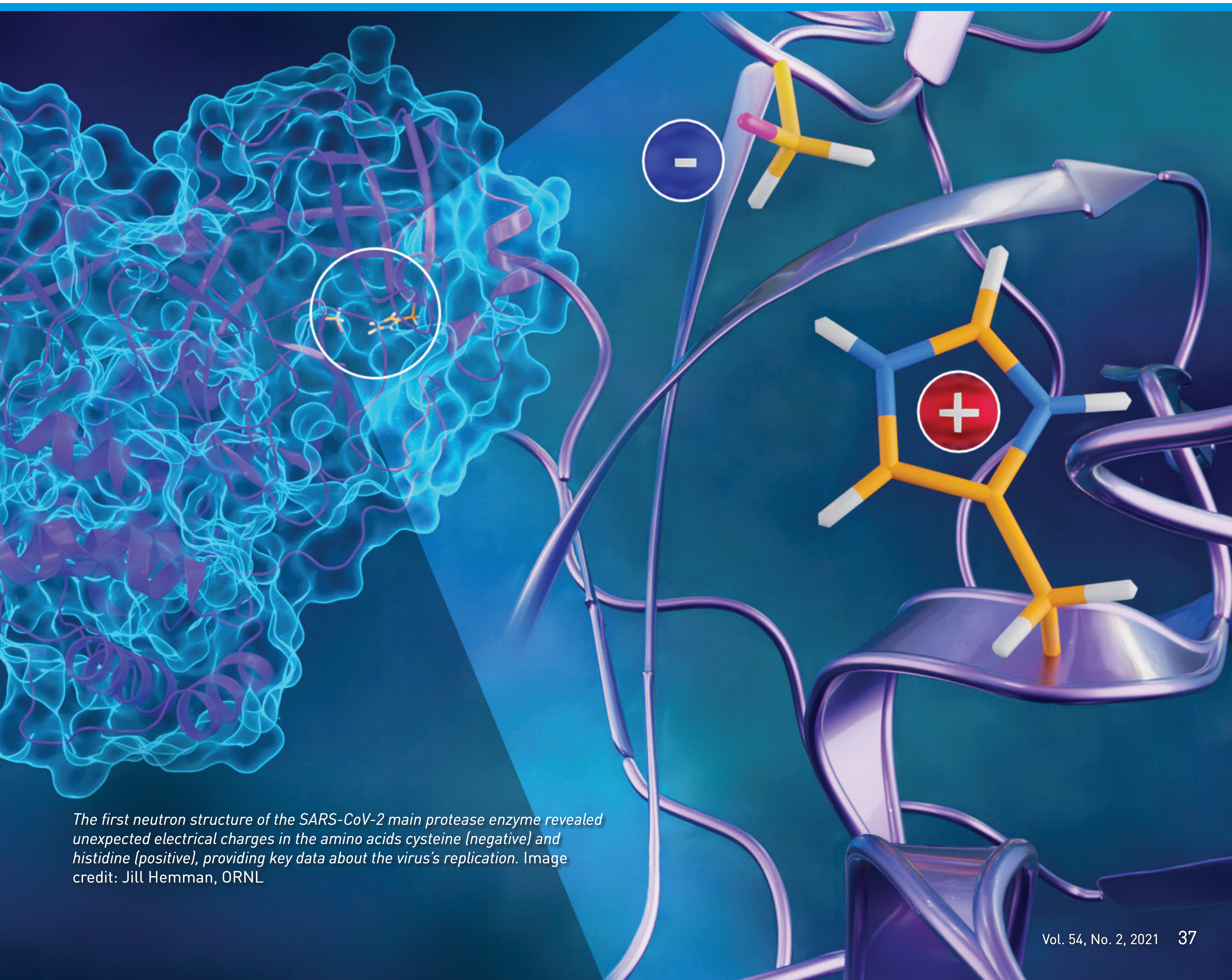
The team's neutron study builds on previous research published in the journal *Nature Communications*, creating a complete atomic structure of the protease enzyme. To accelerate solutions to the global pandemic, the researchers also made their data publicly available to the scientific community before both papers were published.

Neutrons are ideal probes for studying biological structures because they are nondestructive and highly sensitive to light elements such as hydrogen. The neutron scattering experiments were performed at the High Flux Isotope Reactor and the Spallation Neutron Source. The protein samples were synthesized at the Center for Structural Molecular Biology.

"This might be the quickest neutron structure of a protein ever produced. We started neutron experiments in May, and within five months we obtained and published our results. That's something that usually takes years," said co-author Leighton Coates, who works with the SNS Second Target Station. "This work demonstrates what we can do at Oak Ridge. Everything was done here from start to finish. The proteins were expressed, purified and crystallized, and all the data was collected and analyzed on site — a completely vertically integrated approach."

The team will now use the newly obtained information to investigate the binding properties of drug molecule candidates to produce improved COVID-19 therapeutics.

"Not only is this the first time anyone has obtained a neutron structure of a coronavirus protein, but it's also the first time anyone has looked at this class of protease enzymes using neutrons," said lead author Daniel Kneller, a postdoctoral research associate in ORNL's Neutron Scattering Division. "It's an outstanding example of neutron crystallography serving the community when it needs it the most."



The first neutron structure of the SARS-CoV-2 main protease enzyme revealed unexpected electrical charges in the amino acids cysteine (negative) and histidine (positive), providing key data about the virus's replication. Image credit: Jill Hemman, ORNL

Neutrons probe

cell membrane defense against COVID-19

by Olivia Trani
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A cell's membrane is its outermost defense against the novel coronavirus responsible for COVID-19.

Researchers from Virginia Tech and ORNL are using neutron scattering to investigate how the cell membrane and the virus interact with each other and what therapeutic candidates could make cell membranes more resistant to viral entry. Such information could help experts design strategies for slowing down the progress of viral infection and reducing its harmful effects.

"Developing treatments that interfere with the viral infection process could help reduce the severity of the COVID-19 disease and enable people to recover more quickly," said John Katsaras, a biophysicist and neutron scattering scientist at ORNL. This, in turn, could decrease the number of hospitalizations and reduce the risk of overwhelming medical facilities.

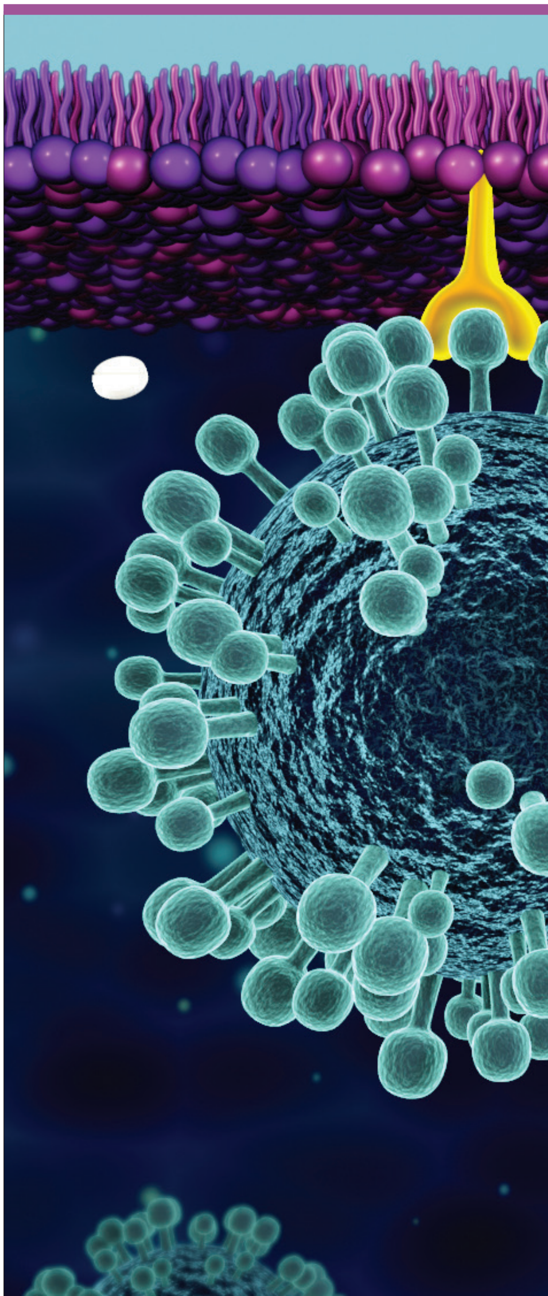
The coronavirus hijacks human cells with the help of spike proteins that protrude from its own membrane layer. The spike protein attaches to the cell surface and helps merge the viral and cellular membranes. Once the membranes are fused, the virus can enter the cell and create copies of itself, spreading the infection throughout the body.

Many researchers are exploring ways to combat the virus by targeting its spike proteins, but fewer are paying attention to the site where the infection process begins: the cell membrane.

"We want to understand how the spike protein interacts with the membrane and what treatments could indirectly block this interaction by targeting the properties of the membrane," said Rana Ashkar, a Virginia Tech physicist and former ORNL Shull Fellow who is leading the research effort.

She collaborated with researchers at ORNL to establish a molecular understanding of the membrane properties that allow viral entry, how membranes change when in contact with the virus and what membrane modifications could inhibit the infection process.

"At ORNL we are able to work with experts from many fields, such as physics, chemistry and biology," said Jessy Labbé, an ORNL cellular and molecular geneti-



cist. "We applied this combined knowledge to develop research projects that address some of the biggest challenges related to the pandemic."

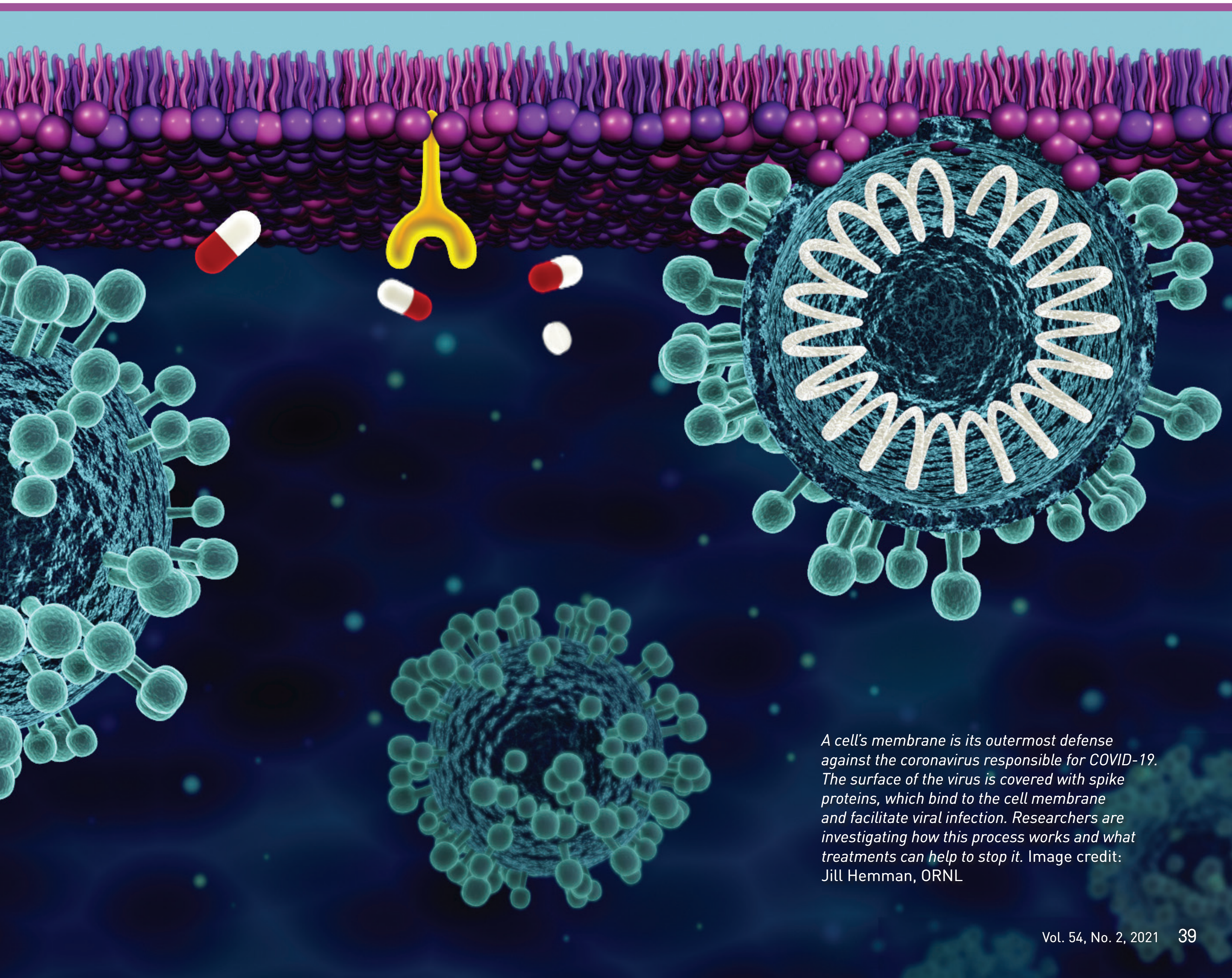
The team is conducting neutron scattering experiments with the liquids reflectometer — or LIQREF — at ORNL's Spallation Neutron Source to examine how membranes and viral spike proteins change their shape upon interaction, as well as the effects of certain therapeutic candidates.

"Using this technique, we can capture the membrane's structure and assess what molecular details change, under physiological conditions, when a membrane is in contact with spike proteins or therapeutic compounds," said Minh Phan, a postdoctoral research associate at ORNL.

The researchers performed their experiments with a membrane model that closely mirrors the shape and composition of cell membranes within human lungs, where respiratory viral infections primarily take place. Using LIQREF, the team first characterized the membrane's original structure. Then they measured how the membrane's properties change when exposed to either melatonin or azithromycin — commonly available products that are being investigated by medical experts as possible treatments for mitigating COVID-19 symptoms.

The team will incorporate viral spike proteins into the membrane samples and analyze various factors of the protein–membrane complex. These include how the spike protein binds to the membrane, the protein's insertion mechanism and the membrane's response to the protein, such as changes to its compression or stiffness. The team will then examine whether these interactions are disrupted in the presence of the therapeutic candidates.

The researchers suggest these methods could be used to rapidly screen various treatments for their potential to help mitigate both the current pandemic and other viral respiratory threats that may arise in the future.



A cell's membrane is its outermost defense against the coronavirus responsible for COVID-19. The surface of the virus is covered with spike proteins, which bind to the cell membrane and facilitate viral infection. Researchers are investigating how this process works and what treatments can help to stop it. Image credit: Jill Hemman, ORNL

ORNL welcomes

by Bill Cabage
cabagewh@ornl.gov

Science is a dynamic process. As society's needs evolve, so must the research institutions charged with addressing those needs.

In May 2020, as ORNL was settling in with the rest of the country for the disruption of a long global pandemic, Laboratory Director Thomas Zacharia called on the ORNL community to reimagine itself — to assess and adjust the lab's agenda to best answer the research needs of the coming generation. To achieve this goal, the lab also needed to attract the next generation's best talents and to attain the organizational agility to support them.

ORNL's major directorates are organized with an eye toward specific disciplines: engineering, physical sciences (i.e., chemistry and materials science), computing, neutron science, nuclear science, biological sciences and national security. The associate laboratory directors who lead those directorates are responsible for guiding ORNL's research enterprise.

Zacharia and his leadership team held a comprehensive appraisal of the laboratory's complex organization. This process acknowledged that while the science landscape often undergoes a slow, seemingly tectonic transformation as missions evolve, the map may also exhibit marked change over a relatively short time.

At the same time the leadership team began evaluating its scientific posture, an emergent national reckoning of attitudes toward race, gender and equality likewise had its influence on the Reimagining initiative. Exclusion deprives a research institution of talent and innovation. ORNL, Zacharia said, should be a laboratory that is inviting for all.

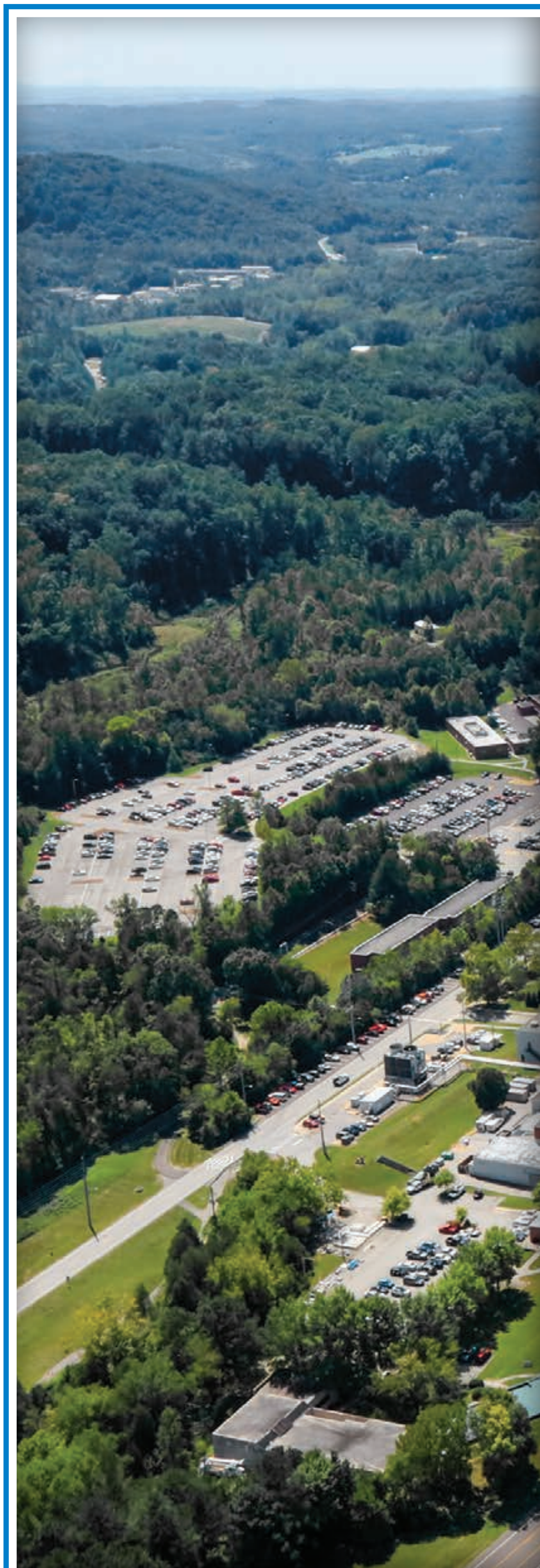
Reimagining ORNL uncovered opportunities to better address the country's most pressing scientific needs. Singular focus on the laboratory's isotopes mission has given its nuclear operations a new momentum. The ultimate reward of fusion energy research and the fission resources within our reach are vital elements of the overall energy economy. Earth sciences and climate research are taking on increasing urgency. And building and transportation engineering hold economic promise as well as environmental importance as the nation assesses a revitalization of its infrastructure.

As a result of this process, the number of the laboratory's research directorates grew from six to eight to allow ORNL to focus more precisely on its goals of becoming the world's premier research institution and supporting U.S. economic growth and national security.

One year later, the lineup of ALDs is much changed from the group that reimagined the lab in 2020. Of the eight ALDs profiled in this section, two are brand new to ORNL. Four are women. Only two have been at ORNL for more than a decade. The new ALDs were selected from across the nation and from extremely competitive pools.

All hail from research and development environments, and all enjoy impressive stature in the scientific community.

We hope you enjoy the following introductions to the scientific leaders who will be guiding ORNL into the future: ALDs Ken Andersen, Deb Frincke, Cynthia Jenks, Kathy McCarthy, Jeff Nichols, Xin Sun, Balendra Sutharshan and Stan Wullschleger. We will be expecting much from them in the coming years.



world-class scientific leaders

Ken Andersen

Solving complicated problems

From Denmark to Japan, the UK, France and Sweden, Ken Andersen has worked at neutron sources around the world. Now, he's leading two American flagship neutron facilities — the Spallation Neutron Source and the High Flux Isotope Reactor — as the associate laboratory director for neutron sciences at ORNL.

"I've always liked working things out, solving complicated problems. Math had sort of a certain glamour, I thought, and it always seemed to me like that's what the clever people were doing. I had a great math teacher in school, and I think that's what inspired me early on."

Andersen earned his B.S. at Keele University in the UK, where he says he fell in love with physics and "messing about with equipment and trying to understand how things work." His years as a Ph.D. student were spent at Keele and the Institut Laue-Langevin — or ILL — in France, where he was introduced to the joys of neutron scattering.

Andersen began his career as a postdoctoral researcher at the National Laboratory for High Energy Physics in Tsukuba, Japan. That's where he discovered his affinity for building instruments.

"At the time, some of the instruments there were sort of held together with sticky tape and string. If you wanted to build anything, you had to physically unstack the instrument, the shielding and the sandbags. You literally had to build the instruments by hand."

For almost 30 years, he's specialized in developing beamlines for user programs at world-leading centers including the ISIS Neutron and Muon Source at Rutherford Appleton Laboratory, UK, the ILL, and the European Spallation Source, Sweden. He joined ORNL as the Neutron Technologies Division Director in 2020. There, he helped guide development of the Spallation Neutron Source's Second Target Station.

As a young scientist at ILL, Andersen learned from the late Otto Schärpf. They worked together on beamline D7, the first instrument in the world to do polarization analysis over a wide-angular-coverage detector. At ISIS, he worked on an instrument project similar to D7, investigating the feasibility of using polarized helium-3 gas instead of polarized supermirrors.

"I chose that instrument project because it pushed the envelope. During my career, I've taken leaps of faith. I believe very much in taking opportunities when they come your way, and considering the opportunities at Oak Ridge in both neutron sciences and the Second Target Station, I'm really pleased I made the jump."

Andersen is married, with three adult children. He's fluent in Danish, French and English, and familiar with Swedish, German and Japanese. Musically inclined, he plays classical piano and occasionally folk music on the violin. He even briefly played the bass guitar — "terribly" — in a rock band with his friends. And, as a runner, you might see the Copenhagen native jogging up Spallation Drive — in the cold, in shorts and a T-shirt.

"I'm very excited about having a part in helping to drive the organization forward. My aim is to lead ORNL's neutron user facilities to the highest possible levels of performance and source availability and help increase their scientific impact even further."

— *Jeremy Rumsey*

Title: Associate Laboratory Director for Neutron Sciences

Research focus: Developing beamlines optimized for user programs

Education: Ph.D., Physics, Keele University, UK

Hobbies: Running, music

Deborah Frincke

Making the world more secure

From an early age, Deborah Frincke has been a keen observer. Her own backyard, teeming with life, was endlessly fascinating, sparking a desire to learn how the world works, and later, how to protect it.

"I believe that making the world a safer, more secure place is rooted in the underpinnings of science," she said. "A better understanding of the digital world and how national security is related to technology will help us arm decision-makers."

Frincke joined ORNL as associate laboratory director for the National Security Sciences Directorate in 2020, tasked with leading and guiding solutions to complex threats that put public safety, national defense, energy infrastructure and the economy at risk.

Prior to her arrival at ORNL, Frincke served in a variety of roles at the National Security Agency, most recently as director of research, where she led what is perhaps the largest in-house research organization in the U.S. intelligence community.

Frincke has become one of the nation's preeminent computer scientists and cybersecurity experts, a path that began at home when her father bought the family a computer. She quickly latched on, taught herself to code and began creating games for her younger siblings. The goal of these geographical map–based games was to keep villages safe.

Later, she completed a bachelor's degree in computer science and mathematics, a master's degree in computer science and a doctorate in computer science, all from the University of California, Davis.

While she was in graduate school, the Morris worm hit the internet, an event that Frincke took as a call to action. "I thought, 'This shouldn't happen. Do something about it.' I did not realize it was going take me the entire rest of my career and my professional life," she said.

After that, cybersecurity became her primary focus. As a postdoc, Frincke founded the University of Idaho's computer security program, which has become a top-ranked national program.

Frincke says she had found her calling. The self-described shy kid was regularly speaking at events and conferences and in classrooms. "I stepped up," she said, "and I did it because I needed to."

She left Idaho for positions at Pacific Northwest National Laboratory and the U.S. Department of Defense. She also served on the Intelligence Community Steering Committee for Artificial Intelligence and the White House Committee on Economic and National Security Implications of Quantum.

Her passion for protecting the nation and its assets will manifest as she continues to hone her vision for NSSD at ORNL.

Title: Associate Laboratory Director for National Security Sciences

Research focus: Cyber resilience and intelligence, geospatial science and human security, and nuclear nonproliferation

Education: Ph.D., Computer Science, University of California, Davis

Hobbies: Rock climbing, bird watching, photography

"The cutting-edge research performed at NSSD leverages deep expertise from not only within our directorate, but also across ORNL, which can be applied to our diverse science areas, from transportation and manufacturing to physics and computing and beyond," Frincke said. "At ORNL, we can have missions that help build and support mitigation strategies to avoid crises before they happen." — *Sara Shoemaker*

Cynthia Jenks

Beyond the surface

Cynthia Jenks leads ORNL's Physical Sciences Directorate with a research portfolio spanning basic and applied initiatives across materials sciences, chemistry, nanoscience and physics. The programs she leads advance understanding of the physical world and drive breakthroughs in new materials, chemical processes and energy technologies.

Jenks says she loves working at the interface of basic and applied research. "It's exciting to see fundamental discoveries about matter and processes build a knowledge base that informs solutions to challenges for energy security, the environment or global sustainability," she said.

Jenks came to ORNL this year from Argonne National Laboratory, where she led the Chemical Sciences and Engineering Division. Prior to her role at Argonne, she directed the Chemical and Biological Sciences Division at Ames Laboratory. Both roles put her at the helm of research activities supported by offices across the DOE, including the offices of Science, Energy Efficiency and Renewable Energy, and Fossil Energy.

An early love of math and chemistry — and great teachers — inspired Jenks to pursue a science career. She studied chemical engineering as an undergraduate but was also drawn to physical chemistry. She earned graduate degrees in both — a master's in chemical engineering and a Ph.D. in physical chemistry — from Columbia University.

The first stage of her nearly 30-year career with the national laboratories began when she was hired as a postdoctoral researcher at Ames. With an expertise in surface chemistry, she probed fundamental questions about the structure and reactivity of surfaces, especially how molecules and surfaces interact. For example, an early project investigated how perfluoropolyethers react with metal surfaces, a chemical process important to high-performance lubricants for the aerospace industry. Jenks' focus on the chemistry of materials has shaped basic research on quasicrystals, intermetallics and metal thin films to advance broad engineering and technology applications.

Her favorite part of working at national laboratories, she says, is the ability to work with scientists and engineers from all areas of expertise.

"That is because the challenges we are working to address as a nation are so big that you need many people with many different backgrounds and perspectives to solve them," she said. "Breakthroughs are often the result of decades of basic research that expands knowledge to make these big questions answerable."

Title: Associate Laboratory Director for Physical Sciences

Research focus: Surface chemistry

Education: Ph.D., Physical Chemistry, Columbia University

Hobbies: Flower arranging, hiking, cooking

As an associate laboratory director, Jenks looks forward to working with DOE to address the nation's energy priorities, ranging from developing energy storage materials, high-performance alloys and plastics, and carbon dioxide capture and conversion to recovering critical materials and exploring the physical processes of cosmic phenomenon.

"We can leverage the expertise of the people and facilities across our directorate and emphasize our unique strengths, such as chemical separations and materials in extremes, to move forward. Tied to that aim, we will continue to expand capabilities at the Center for Nanophase Materials Sciences and engage the lab's neutron resources," Jenks said. — *Ashley Huff*

Kathy McCarthy

Science in the sweet spot

Title: Associate Laboratory Director for Fusion and Fission Energy and Science

Research focus: Liquid metal magnetohydrodynamics

Education: Ph.D., Nuclear Engineering, University of California, Los Angeles

Hobbies: Golfing, hiking, fishing

As the world grapples with climate change, there's never been a more exciting, urgent time to be working in nuclear energy.

"We're perfectly positioned for contributing to clean energy to help us meet those long-term goals," said Kathy McCarthy, associate lab director for fusion and fission energy and science. "We are in the sweet spot."

McCarthy's unique career in fusion and fission seems almost custom-made for this place and time. Over the years, she has gravitated toward the intersections between disciplines, people and ideas, gaining a fresh perspective on issues and building valuable bridges among key players.

After studying fission as an undergraduate, McCarthy shifted to fusion in her graduate studies, researching the use of liquid metals to remove the heat produced by ultrahot fusion plasmas. She worked her way up the research and development leadership ladder at Idaho National Laboratory in a variety of roles. Later, she served as director of Canadian Nuclear Laboratories, where, building on her experience with DOE's Light Water Reactor Sustainability Program, she cultivated ties with industry, translating fundamental nuclear science to power plant operators while absorbing their views and feedback. She is also a member of the National Academy of Engineering.

"That really helped me understand how important practicality is," McCarthy said.

At ORNL, her directorate is accelerating integration and deployment of next-generation fission technology, from concept to industry and regulatory adoption. The directorate is also poised to lead solutions for key science and technology challenges that are essential to economical fusion energy. US ITER provides practical reactor-scale fusion design, fabrication and integration experience for the international ITER fusion reactor in France, while technology-focused experiments such as the Material Plasma Exposure eXperiment, or MPEX, slated to begin assembly in 2023, will support materials studies for post-ITER fusion devices.

"We have the most diverse team of fusion experts that you'll find in the U.S., and unique breadth and integration in fundamental nuclear science," McCarthy said.

Earlier this year, a report from the National Academies of Sciences, Engineering, and Medicine urged the U.S. to move quickly toward developing and building a fusion pilot plant, targeting 2035–2040 for operations. This timeline is driven by the goals of maintaining U.S. fusion leadership and supporting the transition to carbon-neutral energy. Scores of thorny issues must be resolved for that goal: How do we maintain and control "burning" (self-sustaining) plasmas? Can we produce economical fusion power? What exactly is going on in that critical, 10 cm space between the sun-like plasma and the exponentially cooler wall surrounding it?

For these and other issues, ORNL stands at the ready. Said McCarthy, "We envision being the place where the private companies and government come to get their problems solved."— *Kristen Coyne*

Jeff Nichols

Keeping ORNL on top of the computing world

Jeff Nichols leads ORNL's Computing and Computational Sciences Directorate, home to the nation's fastest supercomputer, the laboratory's Artificial Intelligence Initiative and the multi-institutional Quantum Science Center.

The directorate includes DOE's National Center for Computational Sciences, site of the Oak Ridge Leadership Computing Facility. The OLCF delivers transformational scientific research and technological breakthroughs to confront some of the most pressing challenges of the modern era, from the COVID-19 pandemic to climate change to the design of next-generation nuclear power plants.

The OLCF is also home to Summit, the nation's most powerful supercomputer, and will soon host Frontier, which is on track to be the world's first exascale supercomputer, capable of a billion billion calculations each second.

But science is never static, and Nichols is ensuring ORNL remains a global leader by growing programs in quantum computing and networking and evolving the lab's computational portfolio to accommodate the coming data revolution. He is also committed to connecting the lab's experimental facilities with its in-house data analysis capabilities and harnessing the power of artificial intelligence to enable self-driving experiments.

Nichols has led the directorate since 2009. He previously served as deputy associate laboratory director, director of the Computer Science and Mathematics Division and acting director of the NCCS. In those roles, he oversaw the building, installation and deployment of Summit and its predecessors, Titan and Jaguar — each a world leader in high-speed computing — along with supercomputing projects for such clients as the National Science Foundation and DOE.

Prior to joining ORNL in 2002, Nichols was deputy director of the Environmental Molecular Sciences Laboratory at DOE's Pacific Northwest National Laboratory, where he oversaw development, deployment and use of scalable computational science codes to solve grand challenge problems.

Nichols earned a Ph.D. in physical chemistry from Texas A&M University and bachelor's degrees in chemistry and mathematics from Malone College in Canton, Ohio. He has more than a quarter-century of experience as a theoretical chemist and software developer and has written or co-written four software applications and more than 60 research papers.

Title: Associate Laboratory Director for Computing and Computational Sciences

Research Focus: Supercomputing, data science, quantum information science, artificial intelligence

Education: Ph.D., Physical Chemistry, Texas A&M University

Hobbies: Gardening, singing, piano

When he's not advancing the state of the art in computing or blazing new trails in data and next-generation technologies, he enjoys gardening (he recently purchased a greenhouse), cheering on his beloved Michigan Wolverines and playing piano and singing. — *Matt Lakin*

Xin Sun

Leading clean energy transitions through innovation

As the associate laboratory director for ORNL's Energy Science and Technology Directorate, Xin Sun is committed to developing scientific breakthroughs that make the world a better place.

"One of the greatest clean energy challenges facing the world today is how to capture carbon dioxide from the atmosphere and utilize it so that it's no longer harmful to the environment," Sun said. "Contributing to solving problems such as this is at the heart of why I am a scientist, because it's a way to make life better for everyone."

Decarbonization is just one of many initiatives Sun is focused on in her role leading ORNL's largest applied science directorate. With ESTD's expertise in energy generation, transmission, distribution, storage and end use, ORNL aspires to guide the nation to a sustainable, flexible, and secure energy future. ESTD research into advanced manufacturing, building technologies, transportation, and electrification and energy infrastructure presents opportunities for technology advancements such as vehicle electrification, emerging and solid-state batteries, novel materials and processes for additive manufacturing, and equipment for energy efficiency in buildings. Sun said ESTD's emphasis will be not only on research and development for technologies but also on technology demonstration, with the goal of collaborating with industry for commercialization.

"ORNL has historically played a pivotal role in support of Department of Energy missions," Sun said. "ESTD's talented and distinguished scientists are in the right place at the right time to lead the lab in the critical mission of enabling the decarbonization and energy transition. This is a decadal challenge that we are well-positioned to meet."

Sun, who joined ORNL from Pacific Northwest National Laboratory in 2017 as division director for Energy and Transportation Science, is no stranger to solving complex problems. She spent her early career helping to define a new scientific field — computational engineering. She's led the development of complex multi-physics simulations of lightweight automotive materials, joining and manufacturing processes, and developed nuclear materials, carbon capture systems, fuel cells and armor systems. She is also an expert in integrated computational materials engineering. Most recently at ORNL, Sun developed research programs focused on enhanced carbon capture using the lab's strengths in advanced manufacturing and combustion research.

Sun is a fellow of the American Society of Mechanical Engineers and an author of more than 200 journal publications and 10 books. Her research has been recognized with Institute Medals from the American Iron and Steel Institute. She earned a master's degree and doctorate in naval architecture and marine engineering as well as a master's degree in mechanical engineering from the University of Michigan.

"I was attracted to ORNL because of the 'big science' tools, and I look forward to continuing to leverage these resources," Sun said. "We have a huge responsibility within ESTD. We're right in the eye of the storm for change, but this is also the perfect opportunity for staff to shine with their technical capabilities."— *Jennifer Burke*

Title: Associate Laboratory Director for Energy Science and Technology

Research Focus: Decarbonization, carbon capture systems

Education: Ph.D., Naval Architecture and Marine Engineering, University of Michigan

Hobby: Cross-stitching

Balendra Sutharshan

Title: Associate Laboratory Director for Isotope Science and Engineering

Research Focus: Applying isotopes to eradicate cancer and for clean energy

Education: Ph.D., Nuclear Engineering, MIT

Hobbies: Skiing, running, biking

Building an organization of impact

In the mid-1980s, Balendra Sutharshan moved to Canada from the island nation of Sri Lanka.

That move set Sutharshan on a path that had him heading continent-spanning collaborations and holding leadership posts at multiple DOE national labs. In February, he joined ORNL as the associate laboratory director for the Isotope Science and Engineering Directorate.

The directorate is charged with producing unique isotopes for various uses, developing enrichment technology and operating ORNL's nuclear facilities. The broad science portfolio for ISED includes developing ways to make tough-to-produce materials such as plutoniun-238 to power NASA's deep space missions.

Leading such a complex directorate requires expertise and vision. Sutharshan first began developing those qualities not in a radiological lab or at a nuclear reactor, but under the Golden Arches.

"I arrived in Canada and started working at McDonald's, making $4 an hour," Sutharshan said with a chuckle. "It was an experience that gave me the drive to seek the very best education, place my focus into my studies and work toward building the kind of life I wanted."

After completing his undergraduate degree at the University of Toronto, Sutharshan landed at the Massachusetts Institute of Technology to study nuclear engineering. There he witnessed firsthand the life-altering power of isotopes.

While studying boron neutron capture therapy, he helped build a machine for early clinical trials to treat cancer. The goal was to deliver the right isotope to the right target, where it would emit a burst of radiation and kill cancerous cells. Finding the most accurate way to do that was the challenge.

"We know through numerous studies how promising medical isotopes are in treating cancer," he said. "But we've not advanced very far in the last three decades in accurately targeting the tumor site."

After graduating from MIT, he spent nearly two decades at Westinghouse Electric Co., guiding nuclear plant design around the globe. In the process, he said, he experienced many cultures before returning to the U.S. for leadership positions at Argonne and Pacific Northwest national laboratories.

"Thanks to living around the United States and working in nearly 20 countries, I have seen the importance of diversity and inclusion," he said. "If you have the right composition of people — cultivated by an organization that truly believes in diversity and inclusion — it creates an organic and competitive environment that can't be beaten."

Those experiences are already influencing the way he is building ISED. Sutharshan is excited about ISED's existing capabilities and has a compelling vision for expanding the organization's impact.

"If we put our minds to it, we can change the world and develop new ways to use these isotopes — from eradicating cancer to providing clean energy," he said.

"What greater impact is there on society if we can deliver on those promises?" — *Jason Ellis*

Stan Wullschleger

Solving societal challenges through science

Title: Associate Laboratory Director for Biological and Environmental Systems Science

Research Focus: Global change biology, plant ecology

Education: Ph.D., Crop Physiology, University of Arkansas

Hobbies: Community service in urban schools, running

Growing up amidst the cornfields and grasslands of the American Midwest, Stan Wullschleger's fascination with plants bloomed early in life. It was this interest, along with an unquenchable curiosity and love of problem-solving, that led him to pursue a career in science.

Today, Wullschleger heads a unique directorate focused on translating fundamental science into solutions for some of society's greatest challenges — from climate change to clean water to pollution caused by plastics and toxins.

"Tackling big challenges through big science is what ORNL was created to do," Wullschleger said. "We are uniquely equipped to generate the knowledge and the technologies necessary to move the nation toward a brighter, more sustainable future."

As head of the Biological and Environmental Systems Science Directorate, Wullschleger leads a diverse and inclusive organization focused on advancing understanding of the natural world and developing innovations that benefit the environment and grow the nation's bioeconomy. Home to DOE's Center for Bioenergy Innovation, the Climate Change Science Institute and two data centers focused on atmospheric and terrestrial science, the directorate brings together a range of capabilities. Researchers focus on critical goals such as optimizing microbes to convert plastics into valuable chemicals, breeding climate-resilient bioenergy crops and determining which genes allow plants to sequester more carbon.

"Our biggest breakthroughs come when researchers collaborate at the nexus of biology, Earth and environmental science," Wullschleger said. "The multifaceted challenges we're facing today call for an integrated approach that applies discoveries across scales from genes to ecosystems."

This interdisciplinary approach has been a hallmark of Wullschleger's career. As director of ORNL's Climate Change Science Institute and previously as head of the Environmental Sciences Division, he oversaw research that addressed ecosystems, climate modeling and the resilience of environments.

Since 2010, he has also served as director and principal investigator for the Next-Generation Ecosystem Experiments Arctic project, leading a team of 140 scientists from four national laboratories and three universities. Researchers conduct extensive fieldwork in remote parts of Alaska, gathering data to advance Earth system models that predict how thawing permafrost in a warming Arctic will impact regional and global climate systems.

Drawn to ORNL for its reputation, Wullschleger came to Oak Ridge in 1990 as a DOE Alexander Holleander Fellow with a drive to learn the secrets behind the laboratory's distinctive success. Fast forward 30 years, and he now asserts it is the people and the cross-cutting collaboration that are key.

Wullschleger feels privileged to build on ORNL's rich history in the biological and environmental sciences. He is also energized by the scientific challenges at hand.

"Scientific discovery has always been the primary motivating factor in my day-to-day work. It forms the heart of what drives me." — *Kim Askey*

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.

Bryan P. Maldonado Puente

Postdoc, Buildings and Transportation Science Division
Ph.D., Mechanical Engineering, University of Michigan
Hometown: Quito, Ecuador

What are you working on at ORNL?

My research focuses on the control of unstable combustion behavior arising at high-efficiency regimes in internal combustion engines. Predictive control strategies based on machine learning methods could be the key to unlocking advanced combustion modes and reducing the fuel consumption of light-duty vehicles.

What would you like to do in your career?

I would like to continue contributing to the development of more efficient, sustainable and affordable propulsion technologies that satisfy the increased demand for mobility while reducing the effects on climate change for future generations.

Why did you choose a career in science?

I grew up watching science documentaries with my father. It was a matter of time until I had the opportunity to study the laws of physics and the mathematics that described them, which immediately captivated me. As a scientist, I enjoy learning and contributing to the understanding of our natural world.

Yiling Yu

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Physics, North Carolina State University
Hometown: Zhuzhou, China

What are you working on at ORNL?

I am studying the growth mechanism of atomically thin 2D semiconductors. I mainly use optical spectroscopic tools to characterize the material post-growth and unveil what was happening during the growth process. I also use the result to improve the growth process, with the goal of promoting targeted optical properties.

What would you like to do in your career?

I would like to join a university faculty. My research interest is understanding light–matter interactions and engineering the growth of materials to improve their optical functionality. As a teacher, I would like to foster students' interest in research by connecting knowledge and real experiments.

Why did you choose a career in science?

I have had a great interest in science since my childhood. I am always curious about the underlying mechanisms of how things work and why things appear in their current forms in nature. Being a researcher brings me closer to the answer.

Jian Peng

Postdoc, Materials Science and Technology Division
Dr.-Ing., Materials Science, Karlsruhe Institute of Technology, Germany
Hometown: Chibi, China

What are you working on at ORNL?

My research at ORNL focuses on computational materials design by machine learning, high-throughput computing and thermodynamic modeling. I am working on accelerating the design of high-temperature materials (e.g., alloys, ceramics and cermet) and optimizing manufacturing processes such as additive manufacturing and chemical vapor deposition.

What would you like to do in your career?

I would like to stay in academia. I want to use material modeling approaches to deepen our understanding of various high-temperature materials and develop novel materials with improved performance.

Why did you choose a career in science?

Becoming a scientist was the dream of my childhood. I have great curiosities about the unknown world and enjoy the sense of accomplishment in solving scientific problems. I love learning new techniques and knowledge. I hope my research outcomes can make a better life for the world.

Faye Koenigsmark

Graduate student, Environmental Sciences Division
Ph.D. student, Environmental Engineering, Duke University
Hometown: Enfield, Connecticut

What are you working on at ORNL?

I use a combination of benchtop experiments and characterization techniques to understand the speciation of mercury in soils. This knowledge can be used to infer risk of mercury transport from contaminated sites to nearby waterbodies, where mercury may bioaccumulate in fish.

What would you like to do in your career?

Through my research on mercury fate and transport, I've become aware of the inequitable impact of environmental exposures on communities of color and low-income communities. As such, I ultimately want to use my skills in environmental risk assessment and engineering to assist impacted communities in their fight for environmental justice.

Why did you choose a career in science?

I was very concerned about endangered species as a kid. And I think that concern about living things needing a clean, healthy environment to thrive eventually translated into a passion for science.

Jason Hirschey

Graduate student, Building Technologies Office
Ph.D. student, Mechanical Engineering, Georgia Institute of Technology
Hometown: Covington, Washington

What are you working on at ORNL?

I'm working on thermal energy storage systems for space heating and cooling applications. These "heat batteries" complement existing HVAC systems to store thermal energy for air conditioning. By taking advantage of daily outdoor temperature fluctuations, TES-integrated HVAC systems can operate more efficiently and smooth the energy demand curve.

What would you like to do in your career?

The energy industry is changing at an exciting pace. Many people, including myself, feel that it is not evolving urgently enough to minimize the effects of climate change. My goal is to ensure energy equity and contribute to the rethinking of the energy industry by replacing outdated technologies and policies.

Why did you choose a career in science?

Science as a way of thinking is something I have always gravitated towards. I believe data-driven and empirical decision-making is crucial for bettering the world. I have an interest in learning and applying my skills to answer difficult challenges.

Gabriela Schröder

Graduate student, Neutron Scattering Division
Ph.D. student, Biochemistry, North Carolina State University
Hometown: Harrismith, South Africa

What are you working on at ORNL?

I am interested in elucidating the structure of metalloproteins using neutron protein crystallography. Neutrons allow a unique window into the inner chemistry of proteins, since they enhance the visibility of hydrogen atoms. My research is focused on using this knowledge to determine the reaction mechanism by which monooxygenases degrade cellulose and functionalize xenobiotics.

What would you like to do in your career?

Proteins are extraordinary molecules — they are the workhorses of the cell, powering processes and catalyzing a range of essential reactions. I would like to contribute to the understanding of the structure–function relationships and catalytic mechanisms that allow these enzymes to perform their important roles and find new ways to improve them for biotechnological applications.

Why did you choose a career in science?

I have always been inclined to science, particularly trying to puzzle out how things work on the molecular level. Proteins are fascinating machines whose potential can be harnessed for unique chemistry. I enjoy the challenge of solving problems, and delving into the intricacies of protein catalysis has been a challenging but rewarding process.

A piece of aviation history hidden in the woods

by Jim Pearce
pearcejw@ornl.gov

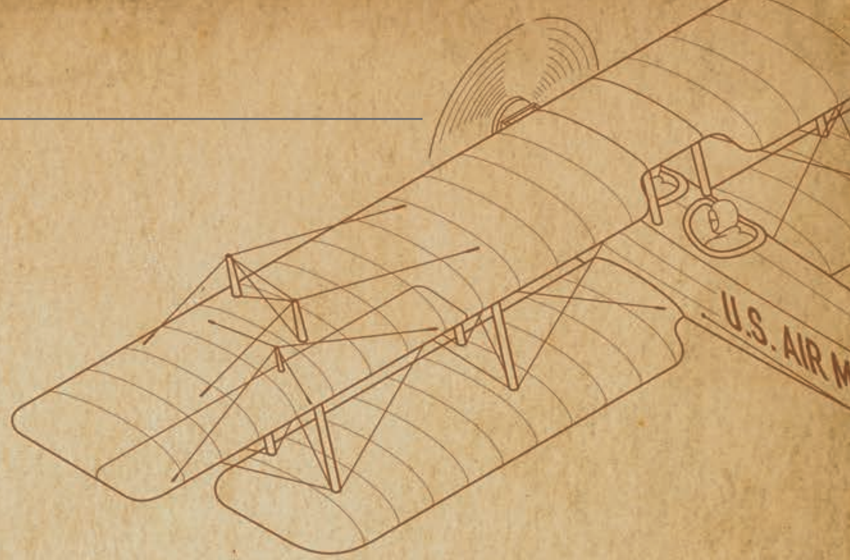
By the time Charles Lindbergh's nonstop flight across the Atlantic electrified the world in 1927, airmail was just becoming commonplace in the United States. In those days, delivering mail by air was not a profession for the faint of heart. Lindbergh himself worked briefly as an airmail pilot not long before his record-setting flight.

While traversing the Atlantic, Lindberg couldn't use landmarks to mark his progress, so he relied on the difficult and sometimes inaccurate technique of "dead reckoning" — navigating with a compass and estimating his location based on speed and elapsed time. Early U.S. airmail pilots, particularly those flying at night or in bad weather, faced similar navigational challenges until the Post Office commissioned the Transcontinental Air Mail Route, a network of airway beacons designed to guide pilots across the largely featureless nighttime landscape.

Each lighthouse-like beacon consisted of a tower topped with a rotating light, a large concrete arrow pointing the way to the next beacon, and a brightly colored shed to house the generator that powered the light. The light produced flashes that could be seen by pilots up to 40 miles away. As a result, after dark or in bad weather, pilots could find their way across the country by flying from beacon to beacon — making airmail delivery a 24-hour operation and dead reckoning over large distances a thing of the past. At its peak in the early 1930s, the airway beacon system included about 1,500 beacons and covered 18,000 miles.

One of these airway beacons was located atop Chestnut Ridge not far from ORNL's Visitor Center. The beacon was constructed

The airmail beacon's generator shed was discovered in 2007 (left) during clearing for an electrical transmission line. It was restored to its original color scheme (right) in 2008. Image credit: Curtis Boles (left) and Carlos Jones (right),ORNL



around 1920 as part of the Knoxville-to-Nashville airmail route. Because the area was relatively remote and primarily agricultural, it is thought that the beacon was maintained by a local farmer. Sometime in the 1930s, the beacon went out of use with the advent of radio navigation. A few years later, Chestnut Ridge and the surrounding land was bought by the federal government for the Manhattan Project, leaving the site undisturbed and eventually hidden by decades of forest growth.

The abandoned site was discovered in 2007 during clearing for an electrical transmission line. The beacon's generator shed, the concrete pad for the fuel tank, and holes in the ground where concrete piers anchored the tower's four legs are all that remain 100 years after the beacon's construction. Presumably, the rest of the equipment was salvaged after the beacon was taken out of service.

In 2008, the site was cleared of brush, and the generator shed's original bright yellow-and-black livery was restored. The effect of the facelift was striking. The brilliantly colored shed with its starkly geometrical black band bursts out of the landscape, giving visitors a sense of how distinctive airway beacons must have been from the air — even in the daylight — and illustrating and preserving a small piece of our nation's aviation history.

Image credit: Brett Hopwood, ORNL

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