OAK RIDGE NATIONAL LABORATORY

Review

Collaborating on climate change:

Oak Ridge National Laboratory

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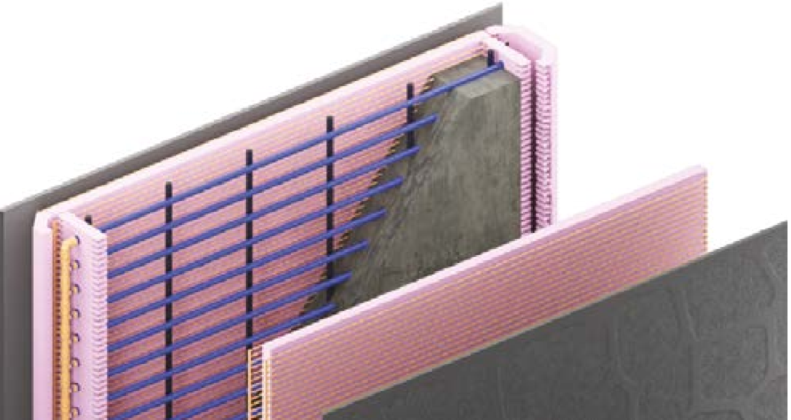


On the Cover
ORNL computational scientist Melissa Allen-Dumas and colleagues connect Earth system models with local decision making. Image credit: Carlos Jones, ORNL

The race to address climate change

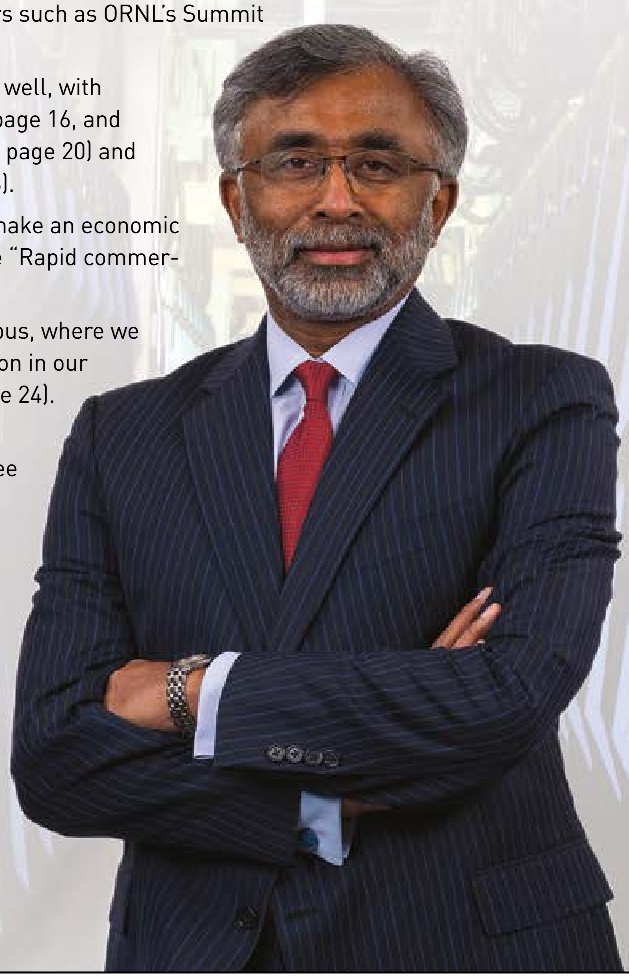
Oak Ridge National Laboratory has always used its unique capabilities, cross-disciplinary collaborations, and public-private partnerships to seek solutions to the most difficult challenges of the day.

In recent years, that has meant engaging the fight against climate change and applying our broad expertise and resources to improving understanding of this most complex of global issues. It is a fight that will require renewed focus and breakthrough science in pursuit of net-zero greenhouse gas emissions by 2050.

The warming climate is bringing us rising sea levels, more severe storms and harsher droughts, with myriad impacts that are less obvious but no less worrisome. Research and development that advances climate science and innovation is a national priority, in fields such as energy storage, carbon capture, biofuel/bioproducts, quantum computing, electric vehicles, grid security, nuclear technology, and many more.

As the Department of Energy's most diverse Office of Science laboratory, ORNL is providing leadership across our broad portfolio, developing scientific tools to better understand our changing world, to predict its future, and to develop the technology that will allow us to live sustainably.

In this issue of *ORNL Review*, we share contributions ranging from research projects in the Alaskan Arctic and the forests of Minnesota to sophisticated models running on world-leading supercomputers such as ORNL's Summit (see "Understanding the complexities of climate change," page 8).



We showcase technological solutions that will help us live both sustainably and well, with improved vehicles and homes (see "New composite revs up vehicle research," page 16, and "Energy efficiency research supports grid-interactive townhome development," page 20) and cleaner industry (see "Novel 3D-printed device enhances CO_2 capture," page 18).

Because new technologies must be deployed to the market to create jobs and make an economic impact, ORNL works hard to engage private industry as quickly as possible (see "Rapid commercialization: Fast tracking promising technologies," page 24).

We also explain our commitment to sustainability on our own 10,000-acre campus, where we focus on native plants and trees in our landscaping and major water conservation in our research facilities (see "ORNL campus becomes a sustainable role model," page 24).

This edition of *ORNL Review* also introduces you to some of the talented young researchers who will ensure our success in the decades to come, including three ORNL scientists who received Early Career Research awards from the Office of Science (see "Celebrating the next generation of great scientists," page 46), graduate students and postdoctoral researchers (see "Why science?" page 50), and the National GEM Consortium that brings talented grad students from underrepresented groups as summer interns (see "GEM Consortium brings talented students to ORNL," page 28).

Finally, we offer an update on how ORNL is applying its considerable resources — including the Summit supercomputer and Spallation Neutron Source — in the fight against COVID-19 (see "Summit simulations uncover COVID-19 connections," page 36, "Neutrons probe cellular invasion processes of COVID-19 infections," page 42, and "Fiber research helps fight COVID-19," page 44).

I hope you enjoy learning about some of the critical work being conducted at ORNL.

Thomas Zacharia
Laboratory Director

Team hits milestone in quantum communication

Few terms are more ubiquitous in the scientific arena these days than "quantum."

Technologies based on the notoriously tricky laws of quantum mechanics promise to enable computers much more powerful than today's fastest supercomputers, unhackable secure communications and unprecedented sensing capabilities necessary for further scientific discovery.

But for these technologies to see the light of day, researchers must develop efficient quantum communications networks that connect quantum devices while preserving the delicate states of the particles used to transmit information.

A team from ORNL, along with colleagues at Purdue University, has taken an important step toward this goal by harnessing the frequency, or color, of light. Such capabilities could contribute to more practical and large-scale quantum networks exponentially more powerful and secure than the classical networks we have today.

Specifically, the team is harnessing the properties of light and the principles of quantum mechanics to transfer information, making the network itself a photonic quantum information processor. This approach is promising for several reasons.

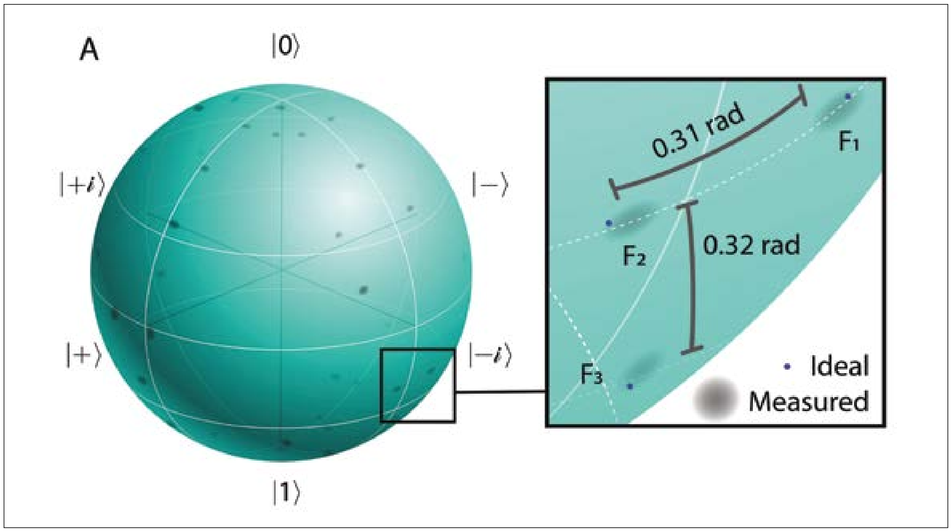
For starters, photons travel at the speed of light, allowing the information to get from point A to point B as quickly as possible. Photons generally don't interact with each other or the surrounding environment, ensuring the information won't become corrupted in transit. "Light is really the only viable option for quantum communications over long distances," said project leader Joseph Lukens.

The team used light to produce frequency-bin qubits, or single photons that reside in two different frequencies simultaneously, to demonstrate fully arbitrary communications operations in frequency encoding for the first time.

Using an ORNL-developed technology known as a quantum frequency processor, the researchers demonstrated widely applicable quantum gates, or the logical operations necessary for performing quantum communication protocols. In these protocols, researchers must manipulate photons in a user-defined way, often in response to measurements performed on particles elsewhere in the network.

By proving that their configuration could transform any qubit state into a different qubit state, the team demonstrated practical information transfer. "If you can do arbitrary operations, you can do any of the fundamental quantum communication protocols such as routing based on frequency conversion," said Lukens. — *Scott Jones*

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



Each point on the sphere of this visual representation of arbitrary frequency-bin qubit states corresponds to a unique quantum state, and the gray sections represent the measurement results. The zoomed-in view illustrates examples of three quantum states plotted next to their ideal targets (blue dots). Image credit: Joseph Lukens and Adam Malin, ORNL

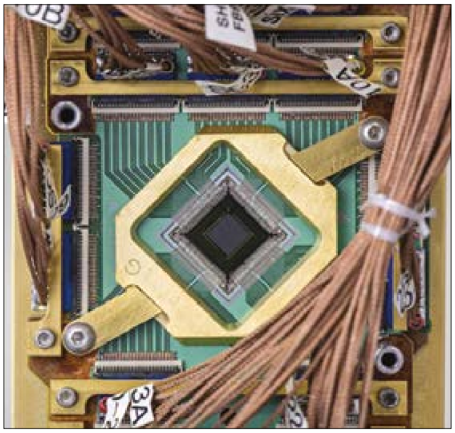
Quantum simulations focus on materials

A multi-institutional team became the first to generate accurate results from materials science simulations on a quantum computer that can be verified with neutron scattering experiments and other practical techniques.

Researchers from ORNL, the University of Tennessee, Knoxville, Purdue University and D-Wave Systems harnessed the power of quantum annealing, a form of quantum computing, by embedding an existing model into a quantum computer.

Characterizing materials has long been a hallmark of classical supercomputers, which encode information using a binary system of bits that are each assigned a value of either 0 or 1. But quantum computers — in this case, D-Wave's 2000Q – rely on qubits, which can be valued at 0, 1 or both simultaneously because of a quantum mechanical capability known as superposition.

"The underlying method behind solving materials science problems on quantum computers had already been developed,



Researchers embedded a programmable model into a D-Wave quantum computer chip. Image credit: D-Wave Systems Inc.

but it was all theoretical," said Paul Kairys, a student at UT-Knoxville's Bredesen Center for Interdisciplinary Research and Graduate Education who led ORNL's contributions to the project. "We developed new solutions to enable materials simulations on real-world quantum devices."

This unique approach proved that quantum resources are capable of studying the magnetic structure and properties of these materials, which could lead to a better understanding of spin liquids, spin ices and other novel phases of matter useful for data storage and spintronics applications. The researchers published the results of their simulations — which matched theoretical predictions and strongly resembled experimental data — in *PRX Quantum*.

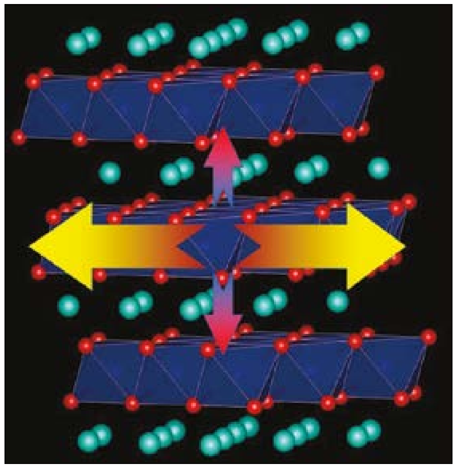
Eventually, the power and robustness of quantum computers could enable these systems to outperform their classical counterparts in terms of both accuracy and complexity, providing precise answers to materials science questions instead of approximations. However, quantum hardware limitations previously made such studies difficult or impossible to complete. *— Elizabeth Rosenthal*

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

Combining bioenergy and carbon capture

The combination of bioenergy with carbon capture and storage could cost-effectively sequester hundreds of millions of metric tons per year of carbon dioxide in the United States, making it a competitive solution for carbon management, according to a new analysis by ORNL scientists.

Bioenergy with carbon capture and storage, or BECCS, uses carbon absorbed by plants from the atmosphere to create energy. Carbon dioxide is captured during the conversion process — such as electricity generation or biofuels production — and stored underground. The result is a negative-emissions technology.



ORNL researchers determined lower heat exchange in lithium-ion batteries is caused by the strong nonharmonic forces among ions and weak interaction between layers, providing guidance for high-density battery design. Image credit: Tianli Feng, ORNL

The ORNL analysis, published in the journal *Land*, confirmed that the approach can sequester from 200 million metric tons per year of CO_2 in the near term to more than 700 million tons per year by 2040. The study pegged the cumulative potential of CO_2 sequestration in the United States using BECCS at 46 billion tons by the year 2100. This represents between 4 and 30 percent of global CO_2 sequestration that could be needed by BECCS by 2100 as outlined in various scenarios by the Intergovernmental Panel on Climate Change.

BECCS is one solution to achieving a limit of a 1.5 degrees Celsius global temperature increase cited by the IPCC, which the panel says is necessary to avoid the most far-reaching impacts of environmental change. BECCS is also cited as part of the solution in a 2018 report of the National Academies Press.

"The research is aimed at improving our understanding of BECCS and informing potential strategies to deal with environmental issues," said ORNL lead investigator Matthew Langholtz. *— Stephanie Seay*

ORNL joins effort to make plastic more recyclable

From soda bottles to car bumpers to piping, electronics and packaging, plastics have become a ubiquitous part of our lives. Advancements in materials have made plastics low cost, flexible, hygienic, lightweight, durable and readily available. While some plastics are recyclable, only a fraction — about 8.4 percent nationally in 2017, according to the Environmental Protection

ORNL's Melissa Tumen-Velasquez works with microbes to understand how the organisms consume plastics and break them into chemical components that can be used to make higher-value products. Image credit: Carlos Jones, ORNL

Agency — is recycled. The vast majority is piling up in our landfills and oceans.

To help address this problem, ORNL researchers are joining the Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment, or BOTTLE, Consortium.

In collaboration with other national laboratories, ORNL scientists will support the development of new plastics that are recyclable by design and customize microbes and processes to break down current plastics into chemical building blocks that can be used to make higher-value products.

These efforts simultaneously aim to reduce waste in landfills and to grow the nation's bioeconomy through renewable generation of valuable chemicals.

ORNL's Adam Guss is leading the effort focused on biological means of upcycling waste plastics into new and more valuable chemicals. Guss, a genetic and metabolic engineer in the Biosciences Division, is developing new tools to modify nonmodel microbes, which are organisms that are difficult to grow in the lab and are not as well studied as model microbes such as *E. coli* and yeast.

"Microorganisms in the environment have an amazing array of genes and metabolic pathways that could be incredibly useful for converting plastics into new chemicals, but many of these organisms have not been discovered yet," Guss said. "By finding these organisms and discovering the genes involved, we can design microbes to convert complex plastic waste into new industrial chemicals."— *Kim Askey*

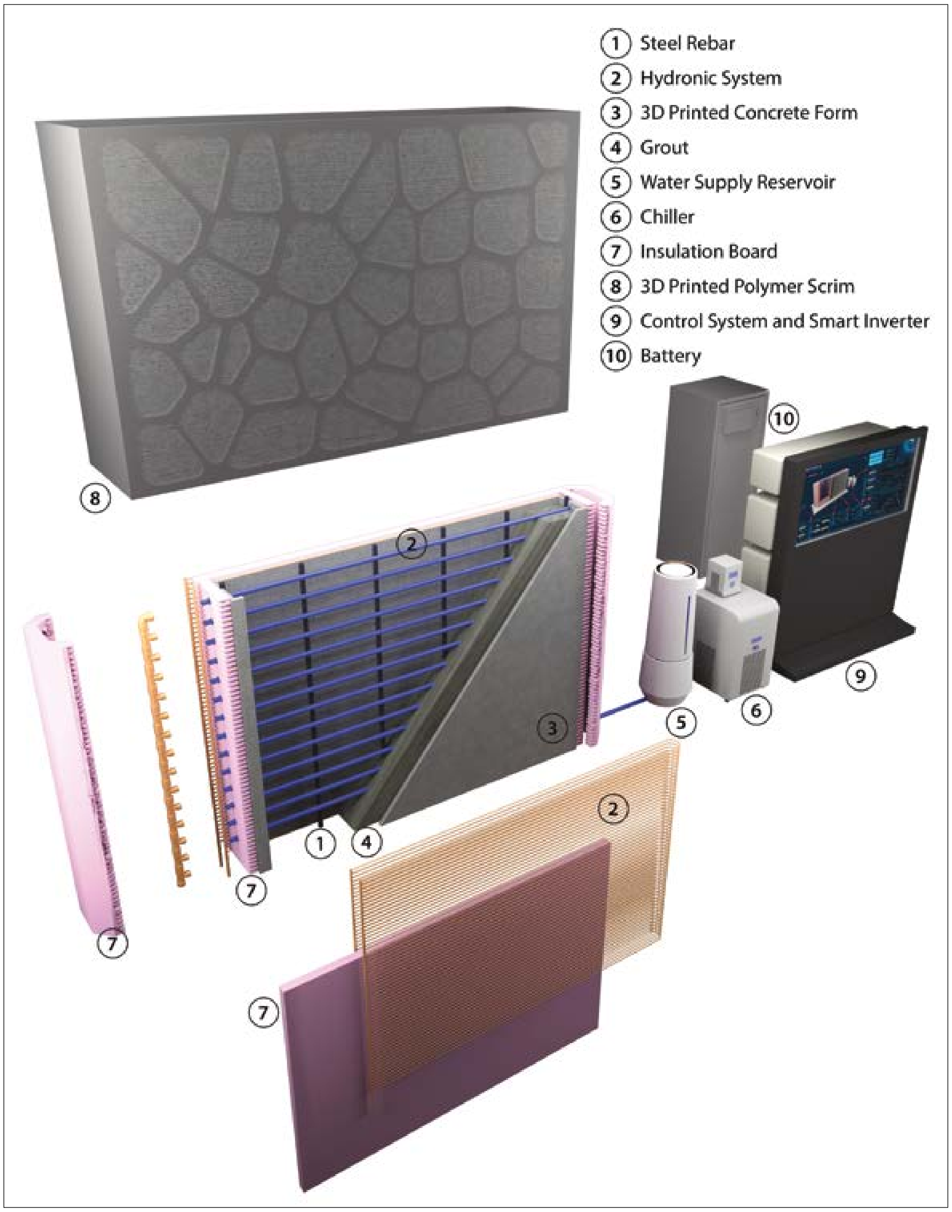
3D-printed smart wall integrates cooling system

A first-of-its-kind smart wall designed by ORNL researchers has demonstrated the future of resilient, efficient and secure next-generation building technology for the DOE's Federal Energy Management Program.

The interior prototype wall, called EMPOWER, measures 5 by 8 feet and allows a room to cool itself without relying on a traditional heating, ventilation and air conditioning system.

The wall was 3D-printed using an additive manufacturing system, SkyBAAM, that is designed to be deployed within hours to any construction site. Driven by cables and calibrated by laser measurements, SkyBAAM dispenses layers of concrete to form complex objects. Using 3D printing facilitates the integration of smart technologies into the wall.

EMPOWER leverages a smart inverter and a chiller that pumps water into the core to cool the concrete. Embedded tubing carries water to and from the chiller, lowering the wall's interior temperature while active insulation controls the wall's surface temperature using the coolness stored in the wall. Model-based predictions control when the insulation is activated, transferring the cool temperature stored in the concrete to the wall's surface through the smart inverter–powered pumps.



The 3D-printed, 5-by-8-foot EMPOWER wall allows a room to cool itself without relying on a traditional heating, ventilation and air conditioning system. Image credit: Andy Sproles, ORNL

The cool surface of the wall reduces HVAC use, while the embedded sensors monitor real-time data to continuously optimize and update the model-based predictions. A battery connected to the smart inverter stores energy from the power grid or from a connected distributed energy source during low-demand times, allowing this energy to be available to lower energy bills, reduce energy consumption and decrease electricity demand without compromising comfort.

"EMPOWER wall's functionality and design can be customized to fit the parameters of the customer and adapted for installation in any building," said Melissa Lapsa, ORNL's Building Technologies program manager. "The overall goal is to reduce energy use, decrease peak-time energy demand, lower energy bills, utilize renewable energy and maintain occupant comfort."

Researchers will validate the technology when an additional smart wall is printed and installed in a building on the ORNL campus in 2021. DOE's FEMP program has collaborated with ORNL to test the smart wall's functionality and will reveal validation results later in the year. *— Jennifer Burke*

Heat resistance of alloys promising for 3D printing

ORNL researchers have demonstrated that a new class of superalloys made of cobalt and nickel remains crack-free and defect-resistant in extreme heat, making them conducive for use in metal-based 3D-printing applications.

Metal materials have proven to be cost-effective for manufacturing, and deploying them for use in additive processes could enable the production of innovative, complex designs with minimal material waste. However, these materials are primarily used in energy, space and nuclear applications that also produce extreme heat environments.

In a study, researchers processed the cobalt and nickel class of superalloys and proved that they remained crack-free in electron-beam and laser-melting 3D-printing processes.

"The challenge has been producing alloys that don't crack in the heat," ORNL's Mike Kirka said. "These superalloys have the material properties necessary for challenging environments, because they not only successfully withstood the heat but also retained strength when stretched." *— Jennifer Burke*

ORNL, Air Force team up on weather forecasting

The U.S. Air Force and ORNL have launched a new high-performance weather forecasting computer system that will provide a platform for some of the most advanced weather modeling in the world.

Procured and managed by ORNL's National Center for Computational Sciences, the system comprises two Hewlett Packard Enterprise, or HPE, Cray EX supercomputers and will primarily support work by the Air Force Weather Wing, which provides the U.S. Army and Air Force with global and regional numerical weather model outputs for planning and executing missions worldwide.

Based at Offutt Air Force Base in Nebraska, the Air Force Weather Wing traces its heritage back to a meteorological service unit in the Army Signal Corps during World War I, and then officially to the formation of the Army Air Force's Weather Wing in 1943. The two supercomputers have been dubbed "Fawbush" and "Miller" after the Air Force meteorologists — Maj. Ernest Fawbush and Capt. Robert Miller — who made the first operational tornado forecast in history at Tinker Air Force Base in 1948.

"Now we have achieved a major milestone in our partnership with Oak Ridge National Laboratory," said Col. Gary Kubat, acting Air Force Weather director. "The delivery of Fawbush and Miller represent a seminal moment in the evolution of Air Force Weather analysis and forecast capabilities.

"Just as Maj. Fawbush and Capt. Miller drove a revolutionary change in military and public weather forecasting, the two halves of this high-performance computing system will open doors to critical new capabilities," Kubat added.

The system's new levels of performance will immediately enable Air Force weather researchers to run their current simulations at a much higher resolution, going from 17 kilometers between model grid points to 10 kilometers, resulting in more precise forecasts. Such weather predictions are vital to the success of military missions around the world. *— Coury Turczyn*

For more information: https://go.usa.gov/xsZ3d

Bienvenue named director of UT–ORNL institute

Joan Bienvenue has been selected as the first executive director of the Oak Ridge Institute at the University of Tennessee, established last year to align the expertise and infrastructure of ORNL and the university in support of world-leading research and talent development. As director, Bienvenue will also serve as a vice provost at UT. She began her new position March 8.

"Joan is a scientific leader with a track record of leveraging university programs and sponsored research to address national priorities," ORNL Director Thomas Zacharia said. "She is perfectly suited to lead partnerships between ORNL and UT that will create long-term national impact, accelerate critical research and prepare our next generation of scientists and engineers."

Bienvenue comes to ORI at UT from the University of Virginia, where she has been senior executive director of the Applied Research Institute — which she launched — since June 2013. As ORI at UT director, she will develop a strategy for establishing leading-edge interdisciplinary graduate research in emerging fields, build world-leading programs that leverage UT and ORNL's capabilities, and lead recruitment of faculty, staff and students.

"Our outstanding faculty, researchers and graduate students are at the heart of the Oak Ridge Institute at UT, and they will no doubt thrive under Dr. Bienvenue's leadership," said UT Knoxville Chancellor Donde Plowman. "Provost John Zomchick, Vice Chancellor Deborah Crawford and I look forward to supporting her in this partnership as the world's leading scientists at both our institutions work together to solve big problems and produce tomorrow's scientists and engineers."

"The opportunity to lead this partnership between a national research university and the country's leading science and energy laboratory holds transformative potential," Bienvenue said. "The institute is a truly visionary initiative that positions UT, ORNL and the state of Tennessee at the forefront of developing the research and talent required to lead the industries of the future. I can't wait to get started."

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

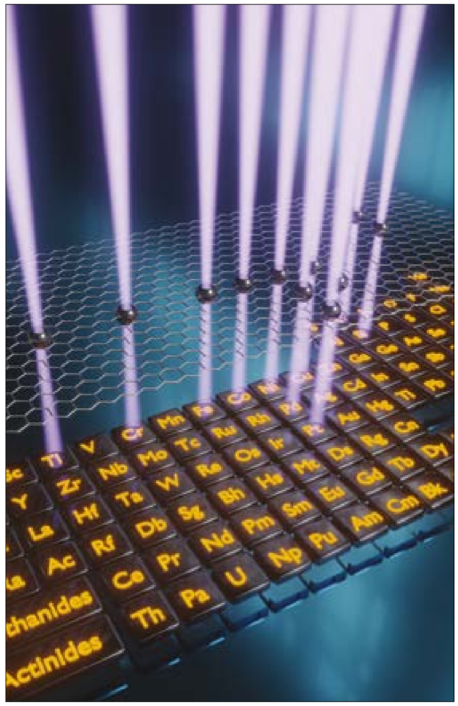
Microscope arranges atoms in graphene

ORNL scientists have demonstrated that an electron microscope can be used to selectively remove carbon atoms from graphene's atomically thin lattice and stitch transition-metal dopant atoms in their place.

This method could open the door to making quantum building blocks that can interact to produce exotic electronic, magnetic and topological properties.

This is the first precision positioning of transition-metal dopants in graphene. The produced graphene-dopant complexes can exhibit atomic-like behavior, inducing desired properties in the graphene.

"What could you build if you could put any atoms exactly where you want? Just about anything," ORNL's Ondrej Dyck said. He co-led the study with Stephen



Transition metals stitched into graphene with an electron beam form promising quantum building blocks. Image credit: Ondrej Dyck, Andrew Lupini and Jacob Swett, ORNL

Jesse at ORNL's Center for Nanophase Materials Sciences.

"If a lot of these quantum building blocks get together, they can start to act in a correlated manner, which is when really exciting properties begin to emerge," Jesse said. The scientists plan to make arrays of interacting quantum building blocks to investigate emergent properties. — *Dawn Levy*

For more information: http://bit.ly/3uJypH6

Breath-sampling whistle for COVID screening

Collaborators at ORNL and the University of Tennessee Health Science Center are developing a breath-sampling whistle that could make COVID-19 screening easy to do at home.

The technology incorporates a unique hydrogel material to capture aerosols from exhaled breath and preserve the samples, which could either be sent to a lab for analysis or, for a fully at-home approach, transferred to an accompanying test kit that could detect the SARS-CoV-2 virus that causes COVID-19.

"Our motivation is to put actionable information in the hands of users to help them make timely decisions, such as whether to go to work or school, quarantine, or seek medical care," said UTHSC's Dr. Scott Strome.

The user-friendly testing format is suitable for a broad range of users, including children and the elderly. The prototype was 3D-printed at ORNL's Center for Nanophase Materials Sciences and designed for low-cost mass production. — *Ashley Huff*

Study shows wildfire's impact on aspen

An ORNL research team has discovered that aspen saplings emerging after wildfire have less diverse microbiomes and more pathogens in their leaves, providing new insights about how fire affects ecosystem recovery.

This study demonstrated, for the first time, the indirect impacts of fire on microbes throughout plant structures.

"The leaves of these saplings never experienced fire, but we were able to show differences in their microbiome compared

Aspen saplings begin to emerge after a fire in June 2019. Image credit: Chris Schadt, ORNL to saplings from unburned areas," ORNL's Chris Schadt said. "Since aspen saplings are clonally derived from the surviving roots, we had thought the leaves might be populated by organisms that were drawn up through the common root. That didn't happen."

The ORNL team plans to further study how microbes repopulate plants after fire. Additional analysis could inform ways to speed vegetative regeneration and the host of benefits that come with healthy forests, from clean water to biodiversity to carbon capture. — *Kim Askey*

For more information:
https://bit.ly/301xl35

Diamond anvil advances neutron research areas

Researchers at ORNL's Spallation Neutron Source have developed a diamond anvil pressure cell that will enable high-pressure science currently not possible at any other neutron source in the world.

Using the facility's SNAP instrument, the team measured high-quality powder diffraction data on a material above 120 gigapascals, shattering the previously held record of 62 GPa for meaningful structural data.

What's more, the tiny submillimeter-sized sample used in the experiment is likely the smallest neutron sample ever measured and yet is also one of the largest powder samples ever held at such a high static pressure.

The diamond anvil pressure cell uses two gem-quality synthetic opposing diamonds to exert extreme pressures on materials, providing fundamental insights into materials that only neutrons can reveal. Image credit: Genevieve Martin, ORNL

While scientists have used X-ray powder diffraction at such pressures for decades, it was previously not possible using neutrons.

"This breakthrough enables new studies on the structures of high-pressure super-hydrides that exhibit room-temperature superconductivity. It even enables investigations into materials at earth-core pressure conditions," said ORNL's Bianca Haberl. — *Jeremy Rumsey*

Welding advance boosts plutonium-238 production

A better way of welding targets for ORNL's plutonium-238 production has sped up the process and improved consistency and efficiency. This advancement will ultimately benefit the lab's goal to make enough Pu-238 — the isotope that powers NASA's deep space missions — to yield 1.5 kilograms of plutonium oxide annually by 2026.

ORNL began using an orbital welder inside a protective glovebox for the weld that closes the hollow tube containing neptunium feedstock — the last step before these targets are irradiated in ORNL's High Flux Isotope Reactor to produce Pu-238.

The new computer-controlled orbital welder produces welds that do not require hand finishing, thereby shortening the time to complete welding jobs from a week to about a day.

"The time saved really adds up as we work toward our production goals," said ORNL's Robert Wham. Plutonium oxide is the power source for Perseverance, NASA's Mars rover. — *Kristi Nelson Bumpus*

ORNL welder Devin Johnson demonstrates a new orbital welder that will make the lab's Pu-238 production program more efficient, by reducing the amount of time it takes to ready hollow feedstock targets for irradiation. Image credit: Carlos Jones, ORNL

Method lowers cost of passive sensors

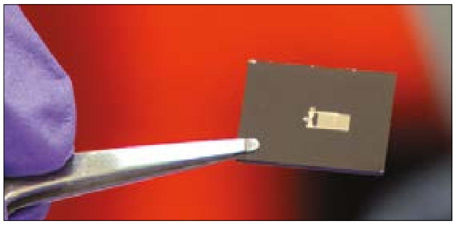
A method developed at ORNL to print high-fidelity, passive sensors for energy applications can reduce the cost of monitoring critical power grid assets.

The sensors use surface acoustic waves, or SAWs, which can pick up changes in temperature, pressure and the presence of gases. In search of a simpler, cheaper alternative to sensors that require elaborate assembly in a clean room, ORNL researchers developed a method to print SAW sensors on substrates of lithium niobate crystal using nanoparticle inks.

The scientists demonstrated that the sensor features can be printed at a resolution of about 10 micrometers, which increases their operating frequency and sensitivity. Ongoing research aims to reach 1 micrometer resolution and to test the sensors in both a simulated nuclear plant application and on essential grid components such as transformers.

"The sensors are low cost, easy to deploy and customizable, and you can make them on the fly," said ORNL's Tim McIntyre. — *Stephanie Seay*

For more information:
http://bit.ly/3c5yxbt



ORNL researchers are developing a method to print low-cost, high-fidelity, customizable sensors for monitoring power grid equipment. Image credit: Carlos Jones, ORNL

Understanding the complexities of climate change

by Kim Askey
askeyka@ornl.gov

With the startling increase in extreme events like wildfires, hurricanes and flooding over the last decade, large regions of the country and the globe are experiencing significant impacts from climate change. Rather than an abstract future possibility, climate change has become a tangible reality — fueling urgency to better understand and predict its effects and develop solutions to address its impact on economic and national security.

The stakes are high. According to the fourth National Climate Assessment — an evaluation written by 300 experts across 13 federal agencies, national laboratories, academia and the private sector — the costs to the United States economy of projected climate effects include $141 billion from heat-related deaths, $118 billion from sea level rise and $32 billion from infrastructure damage by the end of the century.

In the simplest terms, climate change is driven by increasing amounts of carbon dioxide, methane and other greenhouse gases in the atmosphere that trap the heat of the sun and contribute to rising global temperatures.

The reality is much more complex. Myriad interconnected natural and human processes are affecting the accumulation of carbon dioxide and other greenhouse gases. This presents a grand challenge for the scientific community to understand and predict the future of the planet under a range of scenarios and to generate technologies that effectively address environmental change.

As a leader in climate science, clean energy innovations and national security, ORNL is in a unique position to harness extensive expertise and big science tools like the nation's most powerful supercomputer to provide solutions and inform decision-makers tackling this most formidable of challenges.

Advancing a predictive understanding

Understanding the future of our changing Earth begins with intensive investigation into current ecological systems and how they interact. ORNL has been at the forefront of ecology since the 1950s, when the lab began measuring radioactive isotopes in nearby streams. Today, that leadership extends to an array of large-scale experiments in ecosystems that are particularly vulnerable to climate change, from the peatlands of Minnesota to the tropics to the northern reaches of Alaska.

"Our scientists want to understand how the world around us works," said Stan Wullschleger, associate laboratory director for biological and environmental systems science and director of the Climate Change Science Institute. "Fundamental science discoveries are the launch pad for increasingly complex and sophisticated Earth system models."

Improving the predictive capabilities of Earth system models is what drives much of the research. ORNL contributes to a powerful global model known as E3SM, which stands for Energy Exascale

> *"It's been really encouraging to see how much recognition there is across all of these disciplines that everybody has an important role to move this forward as fast as we can.*
>
> — ORNL Earth Systems Science Section Head and Climate Change Science Institute Deputy Director **Peter Thornton**

Earth System Model. E3SM relies on advanced supercomputers such as the lab's Summit system to model fine-scale interactions among land, oceans and atmosphere, including such factors as sea ice and sea levels.

Modeling the carbon cycle — a term that applies to the movement of carbon among the planet's atmosphere, oceans, plants and soils — is an immensely difficult job. Understanding the multitude of processes that influence carbon cycling and coding them into representative equations in Earth system models is often an iterative and collaborative endeavor between teams of scientists collecting data, extracting knowledge and translating that knowledge to the global scale.

Interactions with similar cycles for key nutrients such as nitrogen and phosphorus must be considered as well. Plants store carbon in their roots, stems and leaves, but their growth is often limited by a lack of nitrogen or phosphorus. These elements also affect the pace at which microbes break down organic matter in the soil, releasing stored carbon back into the atmosphere as carbon dioxide.

A team of researchers led by CCSI Deputy Director Peter Thornton, who heads ORNL's Earth Systems Science Section, helped expand E3SM's capabilities to allow coupled simulations of phosphorus, carbon and nitrogen cycles.

"By integrating more process details, we're able to improve predictions of future feedbacks between ecosystems, human systems and climate systems," Thornton said.

Boots on the ground

ORNL is a world leader in investigating these land-based processes at the intersection of biology, chemistry and geology and

See UNDERSTANDING THE COMPLEXITIES OF CLIMATE CHANGE, page 10

ORNL Earth Systems Science Section Head Peter Thornton.
Image credit: Carlos Jones

UNDERSTANDING THE COMPLEXITIES OF CLIMATE CHANGE, page 9

examining their effects on ecosystems. The lab leads two of DOE's flagship projects — NGEE Arctic and SPRUCE — focused on examining the carbon balance in higher latitudes, where temperature is increasing twice as fast as at lower latitudes. These northern ecosystems harbor immense carbon stores in their soil.

ORNL ecologist Verity Salmon.
Image credit: ORNL

Cold temperatures and often water-logged soils in these ecosystems have historically limited microbial activity, slowing decomposition and allowing deep layers of organic matter — and carbon — to build up. With conditions changing, scientists are closely observing shifts in ecosystem patterns through a variety of remote and in-person measurements. Examining data such as rainfall, shrub growth, permafrost thaw, snow depth and the types of microbes found in the soil provides insights into how ecosystem processes are responding to environmental change.

As part of Next-Generation Ecosystem Experiments Arctic, or NGEE Arctic, a diverse team of 150 hands-on scientists and modelers from ORNL, other national labs and universities work together to represent observational data and critical processes in Earth system models.

One such collaboration recently added depth to the representation of plants in Earth system models based on data collected at NGEE Arctic field sites. ORNL ecologist Verity Salmon, ORNL Earth system modeler Ben Sulman (profile, p. 49) and colleagues analyzed the plant data from various watersheds in Alaska and determined which plants should be added to the model as plant functional types — distinct categories of plants with their own parameters and functions to perform in carbon-cycle modeling.

> *"That plant diversity is really functional in this [Arctic] ecosystem. It was exciting to see that structure can be recreated in the model.*
>
> — ORNL ecologist **Verity Salmon**

The research team integrated a representation of lichens, moss and shrubs of different heights into the model and calibrated them to more accurately reflect data on root growth and other key features of Arctic plant life.

"That plant diversity is really functional in this ecosystem," Salmon said. "It was exciting to see that structure can be recreated in the model."

With almost 400,000 types of vascular plants worldwide — those with conductive tissues to move water and nutrients — it is important to get the right representations of crucial plant types in the right locations in Earth system models. There are too many plant varieties to represent them all, so identifying the critical aspects to incorporate is vital.

"It takes a lot of boots-on-the-ground knowledge to decide which factors to represent and to be able to do that appropriately," said Plant-Soil Interactions Group Leader Colleen Iversen, who contributed to the recent study.

Exploring possible futures

What happens when there are important dynamics that cannot be measured because they do not yet exist? ORNL responds by conducting a unique, whole-ecosystem warming experiment that allows scientists to explore a range of possible futures.

Spruce and Peatland Responses Under Changing Environments, or SPRUCE, uses a series of enclosures to expose large peatland plots in the forests of Minnesota to five different temperatures. The hottest of the chambers experiences an increase of about 16 degrees Fahrenheit above and deep below ground. Half the enclosures also receive elevated levels of carbon dioxide.

"Because of DOE's investment in a large-scale experiment, we've been able to study whole ecosystem warming across a range of temperatures that can't be extrapolated from historical data," said Paul Hanson, ORNL Corporate Fellow and SPRUCE project coordinator. "In doing so, we have evidence that carbon losses will be anticipated for rapidly changing peatland systems in the future."

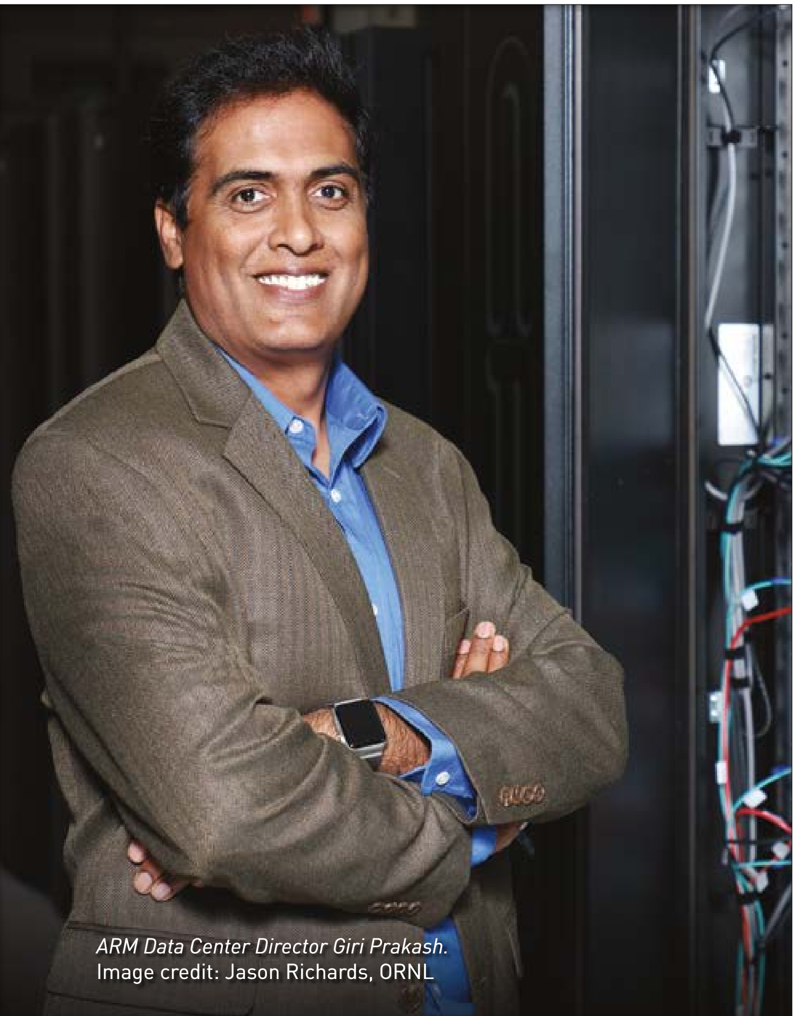
See UNDERSTANDING THE COMPLEXITIES OF CLIMATE CHANGE, page 12

> *“It takes a lot of boots-on-the-ground knowledge to decide which factors to represent and to be able to do that appropriately.*
>
> — ORNL Plant-Soil Interactions Group Leader **Colleen Iversen**

UNDERSTANDING THE COMPLEXITIES OF CLIMATE CHANGE, page 10

Peatlands currently cover around 3 percent of Earth's landmass and hold at least a third of global soil carbon, more carbon than is stored in the world's forests. Peat bogs such as the SPRUCE site are particularly good at locking away carbon because of the cold, wet, acidic conditions that preserve meters-deep layers of ancient plant matter.

ORNL scientists examined three years of SPRUCE data, tracking changes in plant growth, water and peat levels, microbial activity, fine root growth and other factors that control the movement of carbon into and out of the ecosystem. Together, these intakes and outputs make up what's known as the carbon budget.



ARM Data Center Director Giri Prakash.
Image credit: Jason Richards, ORNL

The study found that in just three years, all warmed bog plots turned from carbon accumulators into carbon emitters. This fundamental shift in the nature of the bog occurred even at the most modest level of warming (about 4 degrees Fahrenheit above ambient temperature) and showed carbon loss rates five to nearly 20 times faster than historical rates of accumulation.

Fueling science with data

The SPRUCE and NGEE Arctic projects are slated to continue well into the future, promising to yield additional insights about these changing ecosystems. Volumes of experimental data from the projects are available for use by the broader scientific community, as is the E3SM model. ORNL has long served as a repository and resource for climate-change data, storing measurements from around the world and providing the data in climate model–friendly formats.

Ecosystem and carbon cycle data from ground-, aircraft- and satellite-based campaigns are available through the ORNL Distributed Active Archive Center, which stores and distributes data from NASA Earth Science missions focused on terrestrial systems.

> *"These data are an invaluable resource for scientists to improve predictions of global environmental changes.*
>
> — ARM Data Center Director **Giri Prakash**

Millions of atmospheric measurements of sunlight, cloud characteristics, particles in the air and other phenomena influencing global climate are shared via the ORNL-managed data center for the DOE Atmospheric Radiation Measurement (ARM) User Facility. Sensors from the Americas to the Azores capture these data, with some measurements taken every 10 seconds.

The ARM Data Center hosts 11,000 data products encompassing thousands of terabytes of data, including measurements from the American Midwest and the Amazon, from ships traveling the Southern Ocean between Tasmania and Antarctica and, most recently, from instruments ensconced on an ice floe for a year at the North Pole.

"These data are an invaluable resource for scientists to improve predictions of global environmental changes," said ORNL's Giri Prakash, director of the ARM Data Center.

More knowledge, better predictions

These data inform and help to validate projections from Earth system models, which are often primed by focusing on the last 150 years through the present. Comparing outputs from the model to the actual data for those time periods aids scientists in calibrating the models to better predict future global change.

"We want models in which we can have the most assurance," said Forrest Hoffman, group leader for Computational Earth Sciences. "We always run over the historical period, and that gives us a lens through which to look at future projections."

Many climate models are in use, and each has its own strengths and sensitivities. Hoffman leads an international benchmarking project focused on comparing models to quantify aspects where one model does better than another. The project aims to reduce

uncertainty and variation in the model results. "Using a wealth of truthful data," Hoffman says, "we are in pursuit of the Truth with a capital T."

Models have improved significantly over the last two decades as new measurement and storage capabilities have yielded increasing amounts of data along with the computing power to analyze and incorporate them. Wullschleger describes this trajectory as moving from the black box models of the past, where the workings of the equations within the models were not transparent, to new models with much richer processes represented.

"When we need to make a decision, or implement some sort of a management strategy, or try to understand, for example, whether planting trillions of trees would make a difference to the global carbon cycle, we can answer that question," Wullschleger said. "Twenty years ago, we didn't have the sophistication in the Earth system models to address that question, but we do now."

Global to local decision-making

Outputs from Earth system models can also feed into smaller-scale models designed to examine climate impacts on the national, regional or local levels, providing useful information for decision-makers.

For example, computational scientist Melissa Allen-Dumas and colleagues used outputs from E3SM to set initial and constraining conditions in a weather model that supplied finer detail about the Chicago area. They equipped the weather model with data on the city's urban topography, including building sizes, locations and heights. Using this integrated process, they looked at several scenarios for developing a vacant piece of land adjacent to the southwest section of the Chicago Loop. Their results showed which building geometries would have the greatest cooling effects on the temperatures and resulting energy use in that future neighborhood and for the entire Loop.

See UNDERSTANDING THE COMPLEXITIES OF CLIMATE CHANGE, page 14

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She sees intriguing opportunities for results from these simulations to feed in the other direction as well to inform E3SM and other global models. Machine learning and artificial intelligence approaches could be key to facilitating closer integration.

> *"Our research in the field, laboratory, and collaboration with computational scientists, provides a wealth of foundational data and insightful projections to not only inform decision-making, but to measure outcomes and progress as we move toward a clean, resilient economic future.*
>
> — Associate Laboratory Director for Biological and Environmental Systems Science and Climate Change Science Institute Director **Stan Wullschleger**

"By putting all of these models together in a loose two-way coupling, we can begin to look at the impacts of how decisions made about individual neighborhoods work their way up to affect global climate," Allen-Dumas said.

Exploiting AI for clean energy, carbon capture

Understanding how dynamics change when new decarbonization technologies are factored into the global carbon cycle is tremendously challenging.

ORNL is a leader in clean energy research and development, generating a significant and growing portfolio of early-stage technologies for transportation, buildings, manufacturing and other sectors. From quantifying the carbon-sequestering potential of bioenergy crops to creating new battery technologies for electric vehicles to engineering carbon capture devices that reduce power plant emissions, researchers across the laboratory are focused on translating fundamental science discoveries into technological breakthroughs to increase energy, economic and national security.

Examining the effects of these innovations on the carbon cycle requires estimating how much and how fast carbon worldwide would need to be taken up to meet a goal such as a specific global temperature. It also means understanding how the effects of technologies, such as chemical processes that directly remove carbon dioxide from the air, would scale over a large geographic area.

The net effect of removing carbon from the atmosphere will not simply be one number subtracted from another. The inter-

ORNL Associate Laboratory Director for Biological and Environmental Systems Science Stan Wullschleger. Image credit: ORNL

> *"We want models in which we can have the most assurance. We always run over the historical period, and that gives us a lens through which to look at future projections.*
>
> — ORNL Computational Earth Sciences Group leader **Forrest Hoffman**

action will be far more complex, with the land and ocean likely releasing carbon into the atmosphere to bring the three systems into balance. This would be a reverse of the process seen in recent years, as the ocean and land have been absorbing much of the excess carbon dioxide from the atmosphere.

This is an area of modeling that ORNL's Thornton and colleagues are just beginning to explore. It pushes the boundaries of predictive understanding. The lab will pave new ground by combining economic and technological factors into Earth systems models — factors such as resource availability and global markets for products that can be made from captured carbon.

"It's been really encouraging to see how much recognition there is across all of these disciplines that everybody has an important role to move this forward as fast as we can," Thornton said.

The model will need to be repeated for each new technology developed. Thornton and his team will build on ORNL's expertise in artificial intelligence to accelerate the research. Using machine learning strategies, the group will identify the parameters that are most important to improve the certainty of model projections.

"What drives us is new insights that, frankly, would not be available to us if we were just doing our small thing by ourselves," said Eric Pierce, division director for Environmental Sciences. "There is a richness in the discoveries at the intersection of these many disciplines that continues to move us forward as individuals and as a broader science community."

"Our research in the field, laboratory, and collaboration with computational scientists provides a wealth of foundational data and insightful projections to not only inform decision-making, but to measure outcomes and progress as we move toward a clean, resilient economic future," Wullschleger said.

New composite revs up electric vehicle research

by Stephanie Seay
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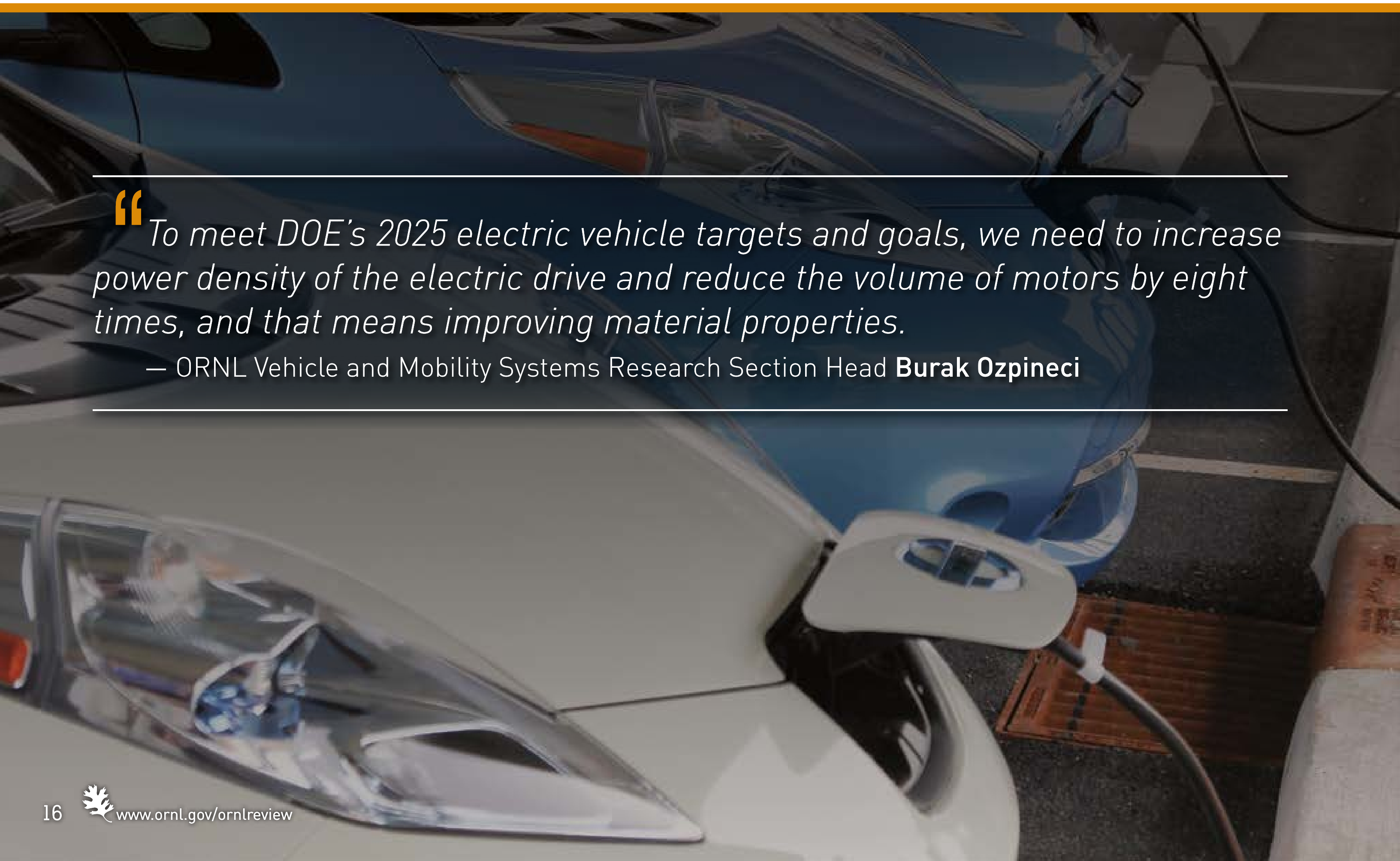
In the pursuit of electric cars with better range and lower cost, researchers have sought improvements to every inch of the vehicle, from a lighter-weight chassis to more energy-dense batteries. ORNL scientists recently contributed a new material to the cause, creating a method to produce a composite that is both lighter and better at conducting electricity than standard electric motor components.

Scientists have long sought to increase the conductive capacity of copper wires without adding extra weight. ORNL researchers turned to carbon nanotubes, or CNTs, which are nanometer-sized tubelike structures made of carbon that are lightweight and 10 times stronger than steel, with exceptional electrical conductivity. Scientists deposited CNTs on flat copper substrates, producing a metal–matrix composite material with better current-handling capacity and tensile strength than copper alone.

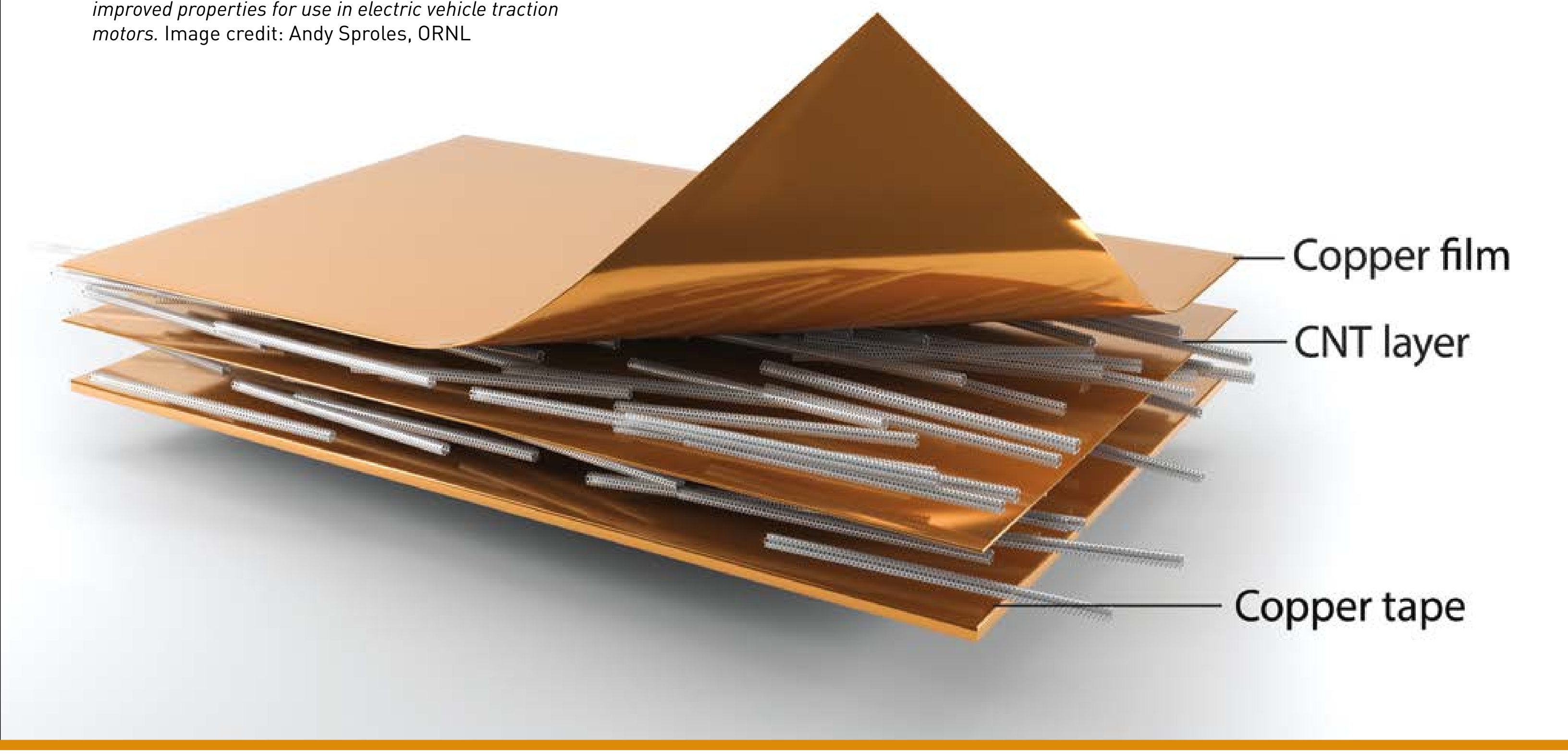
Previous attempts by others to join CNTs and copper had resulted in materials that were only micrometers or millimeters



"To meet DOE's 2025 electric vehicle targets and goals, we need to increase power density of the electric drive and reduce the volume of motors by eight times, and that means improving material properties.

— ORNL Vehicle and Mobility Systems Research Section Head **Burak Ozpineci**

ORNL scientists used new techniques to create long lengths of a composite copper–carbon nanotube material with improved properties for use in electric vehicle traction motors. Image credit: Andy Sproles, ORNL



long, with limited scalability, or that were longer but performed poorly. To overcome the problem, ORNL researchers deposited single-wall CNTs using electrospinning, a commercially viable method that creates fibers while a jet of liquid speeds through an electrical field. The technique provides control over the structure and orientation of deposited materials, explained ORNL materials scientist Kai Li. In this case, the process allowed scientists to successfully orient the CNTs in one general direction to facilitate the flow of electricity.

The team then used magnetron sputtering, a vacuum-coating technique, to add thin layers of copper film on top of the CNT-coated copper tapes. The coated samples were annealed in a vacuum furnace to produce a highly conductive copper–CNT network.

Using this method, ORNL scientists created a copper–carbon nanotube composite 10 centimeters long and 4 centimeters wide with exceptional properties. Researchers found the composite was able to carry up to 14 percent greater current than pure copper, with tensile strength improved up to 20 percent, making it ideal for ultra-efficient, power-dense electric vehicle traction motors.

The material can be deployed in any on- and off-board component that uses copper — creating more efficient bus bars and connectors, for instance — as well as for applications such as wireless and wired vehicle charging systems.

Project lead Tolga Aytug said that "by embedding all the great properties of carbon nanotubes into a copper matrix, we are aiming for better mechanical strength, lighter weight and higher current capacity. Then you get a better conductor with less power loss, which in turn increases the efficiency and performance of the device. Improved performance, for instance, means we can reduce volume and increase the power density in advanced motor systems."

The work builds on a rich history of superconductivity research at ORNL, which has produced superior materials to conduct electricity with low resistance. ORNL's superconductive wire technology invented in the 2000s was licensed to several industry suppliers, enabling such uses as high-capacity electric transmission with minimal power losses.

"Electric motors are basically a combination of metals — steel laminations and copper windings," said Burak Ozpineci, who leads ORNL's Vehicle and Mobility Systems Research Section. "To meet DOE's 2025 electric vehicle targets and goals, we need to increase power density of the electric drive and reduce the volume of motors by eight times, and that means improving material properties."

Novel 3D-printed device enhances CO_2 capture

by Jennifer Burke
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ORNL scientists have designed and additively manufactured a first-of-its-kind aluminum device that enhances the capture of carbon dioxide emitted from fossil fuel plants and other industrial processes.

ORNL's device focuses on a key challenge in conventional absorption of carbon using solvents: the process typically produces heat that can limit its overall efficiency. By using additive manufacturing, researchers were able to custom-design a multifunctional device that greatly improves the process efficiency by removing excess heat while keeping costs low.

Absorption, one of the most commonly used and economical methods for capturing CO_2, places a flue-gas stream from smokestacks in contact with a solvent such as monoethanolamine, known as MEA, or other amine solutions that can react with the gas.

The research team tested the novel circular device, which integrates a heat exchanger with a mass-exchanging contactor inside an absorption column consisting of seven commercial stainless-steel packing elements. The 3D-printed intensified device was installed in the top half of the column, between the packing elements.

> *"The success of this 3D-printed intensified device represents an unprecedented opportunity in further enhancing carbon dioxide absorption efficiency and demonstrates proof of concept.*
>
> — ORNL Associate Laboratory Director for Energy Science and Technology **Xin Sun**

Additive manufacturing made it possible to have a heat exchanger within the column as part of the packing elements without disturbing the geometry, maximizing the contact surface area between the gas and liquid streams.

"We call the device 'intensified' because it enables enhanced mass transfer, the amount of CO_2 transferred from a gas to a liquid state, through *in situ* cooling," said Costas Tsouris, one of ORNL's lead researchers on the project. "Controlling the temperature of absorption is critical to capturing carbon dioxide."

When CO_2 interacts with the solvent, it produces heat that can diminish the capability of the solvent to react. Reducing this localized temperature spike in the column through cooling channels helps increase the efficiency of CO_2 capture.

"Prior to the design of our 3D-printed device, it was difficult to implement a heat exchanger concept into the absorption column because of the complex geometry of the column's packing elements. With 3D printing, the mass exchanger and heat exchanger can co-exist within a single multifunctional, intensified device," said ORNL's Xin Sun, the project's principal investigator.

ORNL researchers designed and 3D-printed an aluminum device that integrates a heat exchanger and mass-exchanging contactor to enhance the capture of carbon dioxide released from fossil fuel plants and other industrial processes. Image credit: Carlos Jones, ORNL

ORNL researchers Costas Tsouris (left) and Eduardo Miramontes insert the carbon capture device inside an absorption column, which contains commercial stainless-steel packing elements. Image credit: Carlos Jones, ORNL

Embedded coolant channels were added inside the packing element's corrugated sheets to allow for heat exchange. The final prototype measured 20.3 centimeters in diameter and 14.6 centimeters in height, with a total fluid volume capacity of 0.6 liters. Aluminum was chosen as the initial material for the intensified device because of its excellent printability, high thermal conductivity and structural strength.

The prototype demonstrated that it was capable of substantially enhancing CO_2 capture with the amine solution, which was chosen because it is highly reactive to CO_2. ORNL researchers conducted two separate experiments: one that varied the CO_2-containing gas flow rate and one that varied the MEA solvent flow rate. The experiments aimed to determine which operating conditions would produce the greatest carbon capture efficiency.

Both experiments produced substantial improvements in the carbon capture rate and demonstrated that the magnitude of the capture consistently depended on the gas flow rates. The study also showed a peak in capture at 20 percent of CO_2 concentration, with the capture rates increasing from 2.2 percent to 15.5 percent depending on the operating conditions.

"The success of this 3D-printed intensified device represents an unprecedented opportunity in further enhancing carbon dioxide absorption efficiency and demonstrates proof of concept," Sun said.

Energy efficiency research

supports grid-interactive townhome development

by Jennifer Burke
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Neighborhoods in the Southeast continue to become more energy efficient with the support of Oak Ridge National Laboratory. Under a collaborative research and development agreement with Southern Company, ORNL researchers have developed a home energy optimization platform for 46 townhomes in Atlanta's first Smart Neighborhood. The platform optimizes each home's heating, ventilation, and air conditioning and water heating systems, in coordination with rooftop solar and batteries, to minimize costs and maintain comfort.

> *"This is a significant result, especially in the national context, where residential and commercial buildings consume nearly 75% of the nation's electricity use and account for 40% of its total energy.*
>
> — ORNL researcher **Heather Buckberry**

This is the second Smart Neighborhood project ORNL has provided research and development support for. The first, with Alabama Power and Southern Company, was completed in 2018 and features 62 state-of-the-art homes connected to a residential microgrid that houses battery and solar energy capabilities.

The Georgia neighborhood, which completed construction in late 2020, differs from the Alabama neighborhood in that each townhome is equipped with solar panels and a battery pack, rather than having those components located at a centralized microgrid. The Georgia homes are equipped with automatic transfer switches that allow essential loads in the homes (refrigerator, lighting, HVAC) to continue operating with battery and solar power in the event of a grid outage. The townhomes are also equipped with electric vehicle charging stations.

ORNL has leveraged DOE's VOLTTRON platform as the framework supporting the ORNL code to optimize the home loads. ORNL's system interacts specifically with the home's HVAC and water heating systems. Using the algorithms developed by ORNL researchers, the system can forecast and optimize the townhomes' energy use in response to signals from the utility.

The Atlanta area townhomes are in Georgia's first Smart Neighborhood, developed by Georgia Power. ORNL is a research partner in the project, managing the homes' energy optimization platforms. Image credit: Southern Company

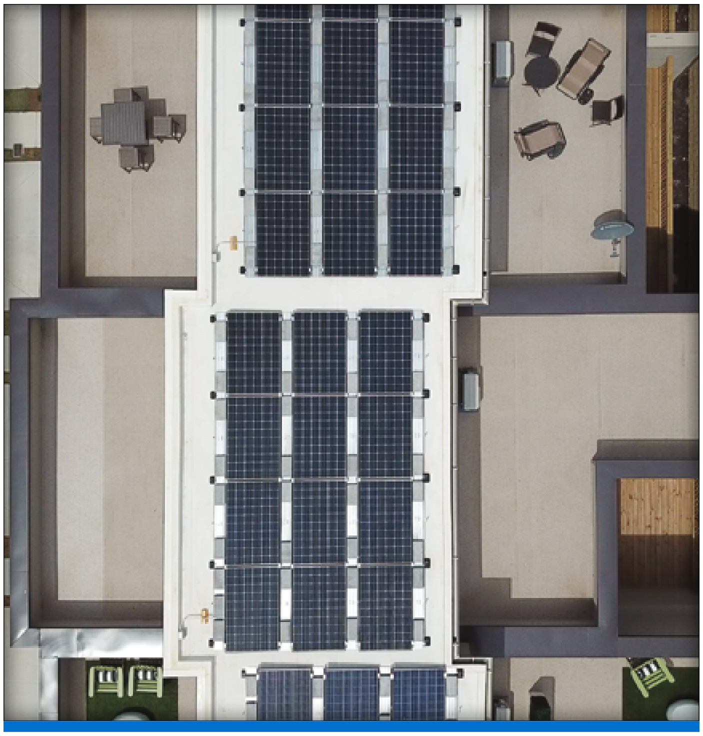
"The process of data gathering, optimization and control happens seamlessly for the homeowner," said ORNL's Heather Buckberry, project manager for both the Georgia and Alabama neighborhoods. "All the homeowner has to do is set the appliances to their comfort level and the system takes care of the rest, providing an efficient, economical and reliable energy source."

Battery storage systems within each townhome provide resilience as a backup power source available for critical loads. The battery systems also maximize the value of the rooftop solar panels by allowing storage of excess power generated during the daytime for use in the evening. Georgia Power anticipates the panels will produce approximately one-third of the homeowner's annual energy usage.

"We're comparing two approaches with the two neighborhoods to test how appliances within homes can be connected to each other and a microgrid and how that interaction can reduce energy usage, while maintaining comfort and affordability," Buckberry said.

Recently published research results on the Alabama Neighborhood showed that the homes consumed 44 percent less energy than all-electric homes, and the peak winter heating electric demand was about 34 percent less than that for a similar all-electric community.

"This is a significant result, especially in the national context, where residential and commercial buildings consume nearly 75 percent of the nation's electricity use and account for 40 percent of its total energy," Buckberry said.



Georgia Smart Neighborhood townhomes are equipped with solar panels that can be used in the event of a power grid outage. Image credit: Southern Company

Both projects provide data on what connected neighborhoods of the future could look like and how future buildings need to communicate with each other and with the grid for shared comfort, efficiency and value.

ORNL's connected neighborhood research is supported by the Department of Energy's Building Technologies Office.

The garages in the multiple-story Georgia Smart Neighborhood townhomes in Atlanta feature an energy storage platform and wireless charging for vehicles. The platform connects to water, heating and air conditioning appliances in the homes and then to a residential microgrid for energy efficiency. Image credit: Southern Company

ORNL campus

becomes a sustainable role model

by Leo Williams
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ORNL is not only the largest national laboratory within DOE's Office of Science, with 5.8 million square feet of facility space. It's also one of the country's oldest national laboratories, with some buildings dating to the 1940s.

As such, ORNL's campus presents a unique opportunity to model campus sustainability by using energy and water efficiently and minimizing the generation of waste and other forms of pollution. ORNL's Carbon-Free Campus plan will integrate carbon capture, energy storage, and emission-free energy technologies to achieve net zero emissions within a decade.

The lab's sustainability efforts are coordinated by Sustainable ORNL, a 12-year effort to ensure that the lab itself is as environmentally responsible as possible. The program encompasses a dozen specific areas — known as roadmaps — such as energy efficiency, a sustainable vehicle fleet, recycling and intelligent building analytics.

"There are multiple areas where we can be sustainable," said ORNL energy and efficiency sustainability engineer Amy Albaugh, "from getting Energy Star–rated equipment to recycling to managing land, energy and water. What Sustainable ORNL does is to bring together all of those areas."

These efforts led to three significant awards in 2020, focused on water savings, the lab's arboretum and personal accomplishments.

Saving water. ORNL's Facilities Management Division saved more than 56 million gallons of water a year in 2018 and 2019 by replacing the source of cooling water to two major research buildings. This effort earned the lab a 2020 DOE Sustainability Award for Outstanding Sustainability Program/Project.

Laboratory equipment in Buildings 4508 and 6000 had connected to ORNL's potable water system using once-through cooling, where the water passes through the equipment once before being sent to the lab's storm sewer. The two-year project hooked the equipment into a recirculating chilled water system, thereby reducing water use in the two buildings by 71 percent.

The 26-acre ORNL Arboretum was accredited in 2019 and contains 52 of the 62 tree species identified at ORNL. Image credit: ORNL

The project added to ongoing Sustainable ORNL efforts pursued by ORNL's Mechanical Utilities to reduce water consumption by repairing leaks and replacing old water distribution lines.

ORNL Arboretum. For years, ORNL has focused on landscaping with native plants and trees, taking advantage of East Tennessee's native beauty and minimizing the use of water and fertilizer in landscaping.

The ORNL Arboretum is an extension of that effort. The 26-acre arboretum, located in the lab's west campus area, contains 52 of the 62 tree species identified at ORNL. It was accredited in 2019 through the International ArbNet Arboretum Accreditation Program and won a 2020 DOE Strategic Partnerships Award for Sustainability.

For ORNL plant ecologist Jamie Herold, the arboretum serves a dual role: educating staff and lab visitors about the region's rich environment and giving them inspiration to incorporate natural plants and trees into their own landscaping projects.

"This is a showcase model for the rest of the lab, but also it highlights what we've done here," she said.

Sustainability Champion. DOE named Albaugh a Sustainability Champion for her contributions to Sustainable ORNL. As leader of the program's Intelligent Building Analytics roadmap, which uses data collection and analysis to promote efficient use of energy and water, she led the implementation of DOE's 50001 Ready energy management program, using the program's Navigator application.

ORNL was only the third federal location to receive the 50001 certification.

"Amy's knowledge, leadership and passion for sustainability have driven many Sustainable ORNL accomplishments," said Mark Goins, ORNL's complex facility manager. "She possesses all the attributes of a true Sustainability Champion, and ORNL is privileged to have an early-career engineer with her capabilities."

For Albaugh, the lab's sustainability programs, and Sustainable ORNL in particular, are an effective way to take advantage of the talented people at ORNL to accomplish something at home.

"It brings people together in a common group where we can discuss and continue to promote and see where we can be of assistance across multiple areas," she said, "and just basically promote sustainability throughout ORNL."

Rapid commercialization:

Fast-tracking promising technologies

by Jim Pearce
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Readers of *ORNL Review* know that our national laboratories are home to super-cool, state-of-the-art facilities where scientists and engineers develop amazing technologies. Equally important is the role national labs play in boosting the nation's economy by teaming up with business and industrial partners to move these technologies from the laboratory to the marketplace.

"We want to get scientific advances into the hands of our commercial partners as quickly as possible, so taxpayers see a return on their investment," said Mike Paulus, director of technology transfer at ORNL. "Technologies do have a shelf life, so as soon as they emerge from the laboratory, they often have the greatest potential value for industry."

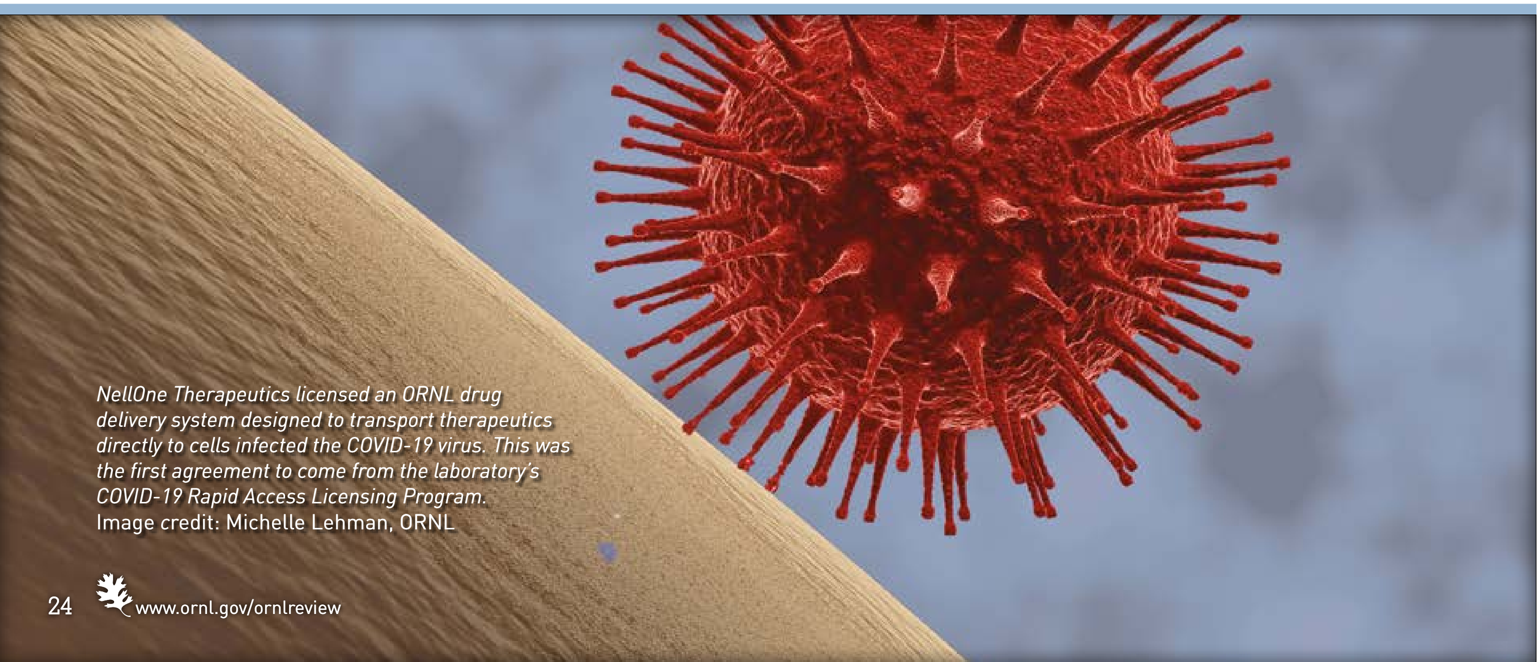
Delivering COVID drugs

One recent example of rapid commercialization was prompted by the COVID-19 pandemic.

Chris Ellis, an ORNL computational microbiologist, developed a drug delivery system that transports therapeutic drugs directly into cells infected by the COVID-19 virus. The system incorporates the virus' spike protein — the part of the virus that enables it to latch onto and infect cells — into the structure of nanoparticles that are filled with doses of an anti-COVID drug. These nanoparticles then bind only to COVID-infected cells and deliver their therapeutic payloads through the cell membrane.

The laboratory licensed this technology to NellOne Therapeutics of Knoxville, Tennessee, for use with the NELL1 protein. This was the first agreement to result from ORNL's COVID-19 Rapid Access Licensing Program.

"The NELL1 protein is useful for treating damage to the heart and lungs, among other things," Paulus said. "We're working with NellOne to adapt the delivery system to transport the NELL1 protein directly to the hearts and lungs of patients whose organs have been damaged as a result of a COVID exposure.



NellOne Therapeutics licensed an ORNL drug delivery system designed to transport therapeutics directly to cells infected the COVID-19 virus. This was the first agreement to come from the laboratory's COVID-19 Rapid Access Licensing Program.
Image credit: Michelle Lehman, ORNL

ORNL computational microbiologist Chris Ellis developed a drug delivery system that transports therapeutic drugs directly into cells infected by the COVID-19 virus. Image credit: Carlos Jones, ORNL

"We licensed this technology to NellOne at no cost," he added. "We're hoping they can quickly develop a tool that will be useful for patients recovering from COVID-19."

Ongoing relationships

Great technology is just the first step to successful technology transfer, Paulus noted. On top of that, the process relies on effective communication between the lab and business partners, to both ensure that potential licensees understand the value of the technology and help guide ORNL researchers to produce the most valuable innovations.

"High-value transfers of technology like this wouldn't happen if we just tossed a technology over the transom and said 'good luck,'" Paulus said. "They occur when we bring our scientific horsepower, our facilities and our person-to-person engagement to bear on a challenge.

"Then the expertise of our industry partner helps to guide our research; our research helps to advance the company; and along the way, inventions result."

A remarkably productive year

The NellOne license is just one of many technology transfer success stories that the laboratory can point to over the last year.

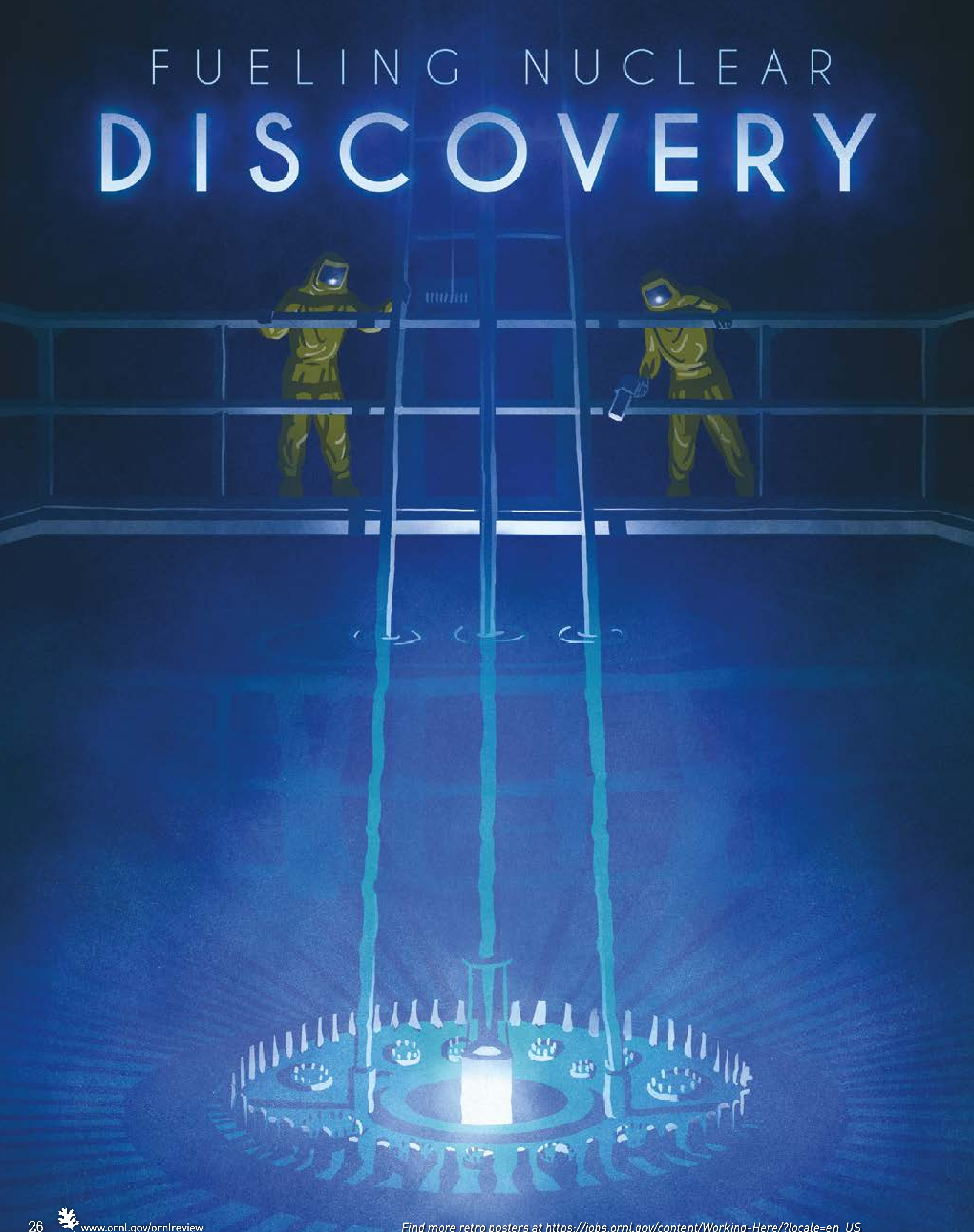
For instance, Texas-based Momentum Technologies Inc. licensed ORNL's Membrane Solvent Extraction process for recovering cobalt and other metals from spent lithium-ion batteries that would otherwise have been discarded. The metals are critically important to manufacturing batteries for everything from the telephones to electric vehicles.

In another successful collaboration, this time in the field of 3D printing, the laboratory licensed a new method of printing collimators — components used in neutron scattering instruments — to ExOne, a company that specializes in 3D-printing technology. That collaboration relied on an ongoing relationship between ExOne and ORNL engineer Amy Elliott.

Collimators help to shape and focus neutron beams. To achieve this, they sometimes have geometries that would be very difficult to create with traditional machine tools, making them an ideal candidate for 3D printing.

These are just a few examples of ORNL licensing successes. The last year has been particularly fruitful for tech transfer, Paulus noted, in spite of the limitations imposed by the global COVID pandemic.

"Our staff has closed more licensing deals than we have in the last 10 years," he said. "That's a testament to how the whole laboratory has stepped up in the face of the pandemic."



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GEM Consortium

brings talented students to ORNL

by Laurie Varma
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In 1989, a handful of ORNL scientists began working with the National GEM Consortium to bring talented graduate students from underrepresented groups to the laboratory as summer interns. Since then, ORNL's partnership with the 44-year-old organization has grown to include 14 research divisions hosting exceptional GEM Fellows.

GEM, a network of leading corporations, government laboratories, top universities and top research institutions, enables qualified students from underrepresented communities to pursue graduate education in applied science and engineering. Students apply for the fellowship through a competitive process, and

ORNL's 2019 GEM Fellows with Moody Altamimi, director of ORNL's Office of Research Excellence (fourth from left) and Michelle Buchanan, former ORNL Deputy for Science and Technology. GEM Executive Director Marcus Huggans and Chief Executive Officer Brennon Marcano (front middle, left and right) stand between Altamimi and Buchanan. Image credit: Carlos Jones, ORNL selected applicants are paired with a GEM employer who sponsors their summer internship.

"Oak Ridge National Laboratory is proud to partner with GEM in our efforts to attract the nation's best and brightest to pursue careers in STEM. It is a privilege and inspiration to engage with these early career scientists and engineers who will shape the future of research and development in our country," said Moody Altamimi, director of ORNL's Office of Research Excellence.

Jeff Nichols, associate laboratory director for ORNL's Computing and Computational Sciences Directorate, points out that diversity of thought and experience leads to diversity of solutions and better research outcomes.

"We can accomplish scientific goals better together than we can alone, so it's a win–win for everyone," Nichols said. "I highly respect the program, and I'll take as many GEM Fellows as we can get.

"We know that if we get a GEM student, they're going to be outstanding," he added. "They have can-do attitudes and the energy and drive to take full advantage of the exceptional resources at ORNL."

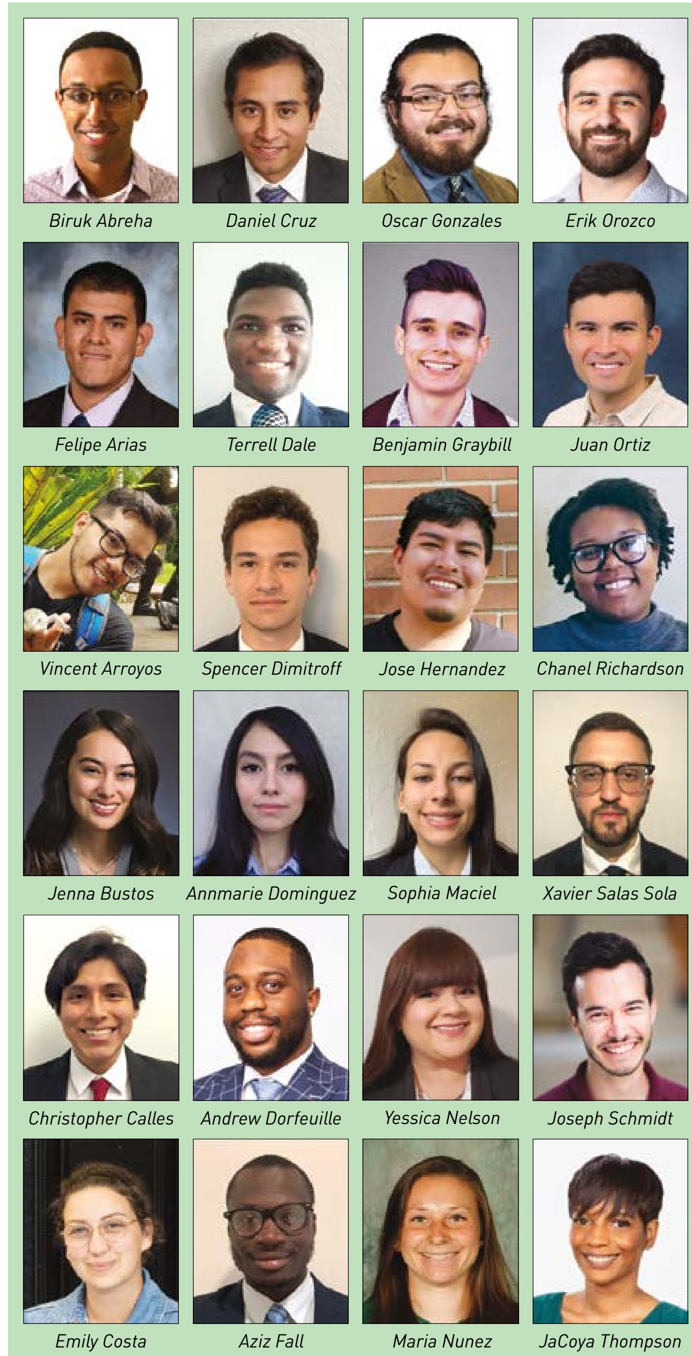
In FY 2020, ORNL selected 24 GEM Fellows — more than double the number for FY 2019 — to intern in summer 2020. Due to the COVID-19 pandemic, the 2020 cohort will be hosted in 2021.

To enrich their research experiences at the laboratory, the ORE has designed sessions for GEM Fellows that help them develop important professional skills, including presentation and communication training and team and community building. In addition, the students are provided the opportunity to network with ORNL staff.

In addition to hosting GEM Fellows in their research directorates, ORNL staff can support the GEM program as an advocate or panelist–judge. In 2020, two ORNL scientists — Hector Santos-Villalobos, Cyber Identity and Biometrics Group leader in the National Security Sciences Directorate, and Candice Halbert, a scientific associate with the Spallation Neutron Source — served as GEM Fellowship advocates, helping expand the laboratory's participation in the GEM program and placing Fellows in research directorates with which their research skills align.

"My experience as an advocate has given me the opportunity to meet, work with, and place hardworking, highly intelligent, multifaceted students," Halbert said. "I look forward to continuing to advocate for GEM. It is an organization that is valuable and needed in the STEM field."

In addition to their service as advocates, in FY 2020 six ORNL staff members served as panelist–judges, helping the GEM organization screen applicants at the national level while also identifying potential candidates for positions at ORNL. In addition to Halbert and Santos-Villalobos, ORNL panelist–judges this year included Valentino Cooper, Materials Theory, Modeling and Simulation section head in the Physical Sciences Directorate; Tiffany Mintz, until recently a software development engineer in the Computing and Computational Sciences Directorate; Christopher Schadt, a research staff member in the Biological and Environmental Systems Science Directorate; and Wei Tian, a neutron scattering scientist in the Neutron Sciences Directorate.



Biruk Abreha · Daniel Cruz · Oscar Gonzales · Erik Orozco

Felipe Arias · Terrell Dale · Benjamin Graybill · Juan Ortiz

Vincent Arroyos · Spencer Dimitroff · Jose Hernandez · Chanel Richardson

Jenna Bustos · Annmarie Dominguez · Sophia Maciel · Xavier Salas Sola

Christopher Calles · Andrew Dorfeuille · Yessica Nelson · Joseph Schmidt

Emily Costa · Aziz Fall · Maria Nunez · JaCoya Thompson

The latest cohort of GEM Fellows will work across the laboratory in research directorates focused on biological and environmental sciences, computing, neutron and isotope science, physical science and national security.

"Being a GEM advocate has been a privilege for me," Santos-Villalobos said. "These students shine hope to the future of our nation and the world."

In recognition of ORNL's efforts in supporting diversity and inclusion, ORNL received the GEM Corporate Award for the first time in 2020. Laboratory Director Thomas Zacharia will accept the award on behalf of ORNL at the national consortium's awards gala in September 2021.

Summit helps

take the guesswork out of drug design

by Rachel McDowell
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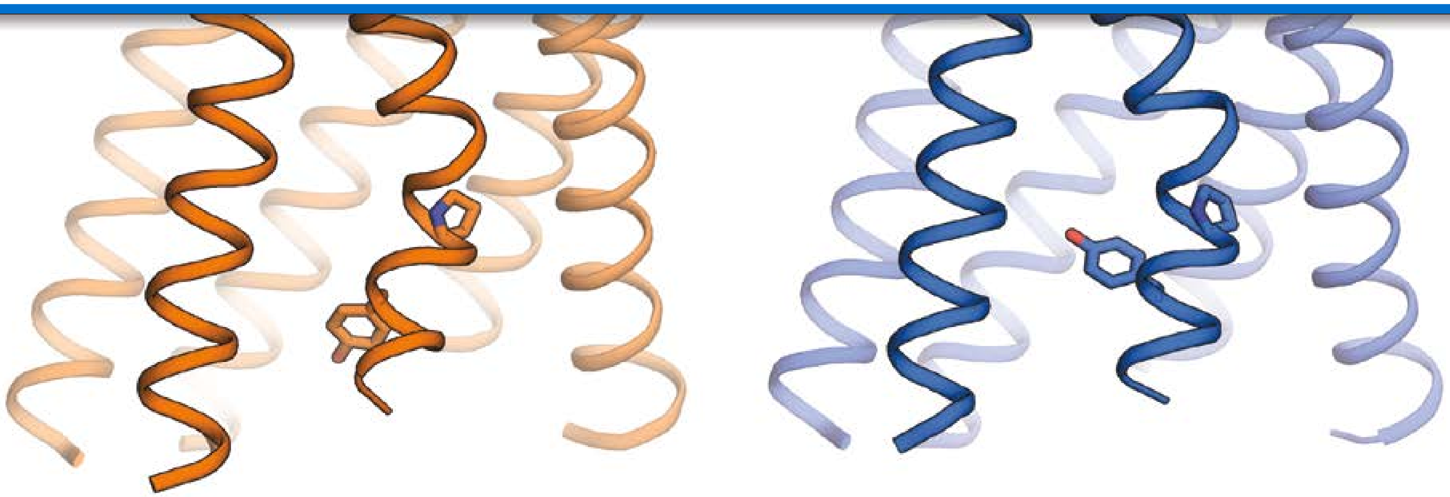
Psychedelic drugs could be effective in treating psychiatric disorders such as depression and post-traumatic stress disorder, but medical use of these drugs is limited by the hallucinations they cause.

"What if we could redesign drugs to keep their benefits while eliminating their unwanted side effects?" asked Ron Dror, an associate professor of computer science at Stanford University. Dror's lab is developing computer simulations using ORNL's Summit supercomputer — the country's most powerful — to help researchers do just that.

In an article published in the journal *Science*, Dror's team describes discoveries that could be used to minimize or eliminate side effects in a broad class of drugs that target G protein-coupled receptors, or GPCRs. GPCRs are proteins found in all human cells. Lysergic acid diethylamide — or LSD — molecules and other psychedelics attach to GPCRs — but so do about a third of all prescription drugs, including medications for allergies, blood pressure and pain. So important is this molecular mechanism that Stanford professor Brian Kobilka shared the 2012 Nobel Prize in Chemistry for his role in discovering how GPCRs work.

When a drug molecule attaches to a GPCR, it can cause multiple simultaneous changes in the cell. Some of these changes



Computer simulations help researchers understand why some drugs cause unwanted side effects. Image credit: Ron Dror, Stanford University might contribute to a drug's beneficial effects, but others can lead to less-than-desirable or even dangerous effects.

Using Summit and a computing cluster at Stanford, the team compared computer simulations of a GPCR with different molecules attached. Dror's team was then able to pinpoint how a drug molecule can alter the way a GPCR's atoms are ordered. Changing the protein's atomic arrangement affects the protein shape and can allow a drug molecule to deliver benefits without side effects — something that has remained mysterious until now. Based on these results, the researchers designed new molecules that were shown computationally to cause beneficial changes in cells without unwanted ones. Although these designed molecules are not yet suitable for use as drugs in humans, they represent a crucial first step toward developing side-effect-free drugs.

Today, researchers typically test millions of drug candidates — first in test tubes, then in animals, and finally in humans — hoping to find a "magic" molecule that is both effective and safe, meaning that any side effects are tolerable. This massive undertaking typically takes many years and costs billions of dollars, and the resulting drug often still has some frustrating side effects.

The discoveries by Dror's team promise to allow researchers to bypass much of that trial-and-error work so they can bring promising drug candidates to animal and human trials faster and with a greater likelihood of success.

Stanford postdoctoral scholar Carl-Mikael Suomivuori and former graduate student Naomi Latorraca led an 11-member team that included Robert Lefkowitz of Duke University, with whom Kobilka shared the Nobel Prize, and Andrew Kruse of Harvard University, Kobilka's former student.

"In addition to revealing how a drug molecule could cause a GPCR to trigger only beneficial effects, we've used these findings to design molecules with desired physiological properties, which is something that many labs have been trying to do for a long time," Dror said. "Armed with our results, researchers can begin to imagine new and better ways to design drugs that retain their effectiveness while posing fewer dangers."

Dror hopes that such research will eventually eliminate the dangerous side effects of drugs used to treat a wide variety of diseases, including heart conditions, psychiatric disorders and chronic pain.

This story was written by Tom Abate at Stanford University and adapted by Rachel McDowell at ORNL.

Supercomputer simulations

explore detonation engines

by Coury Turczyn
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Revisiting an engine concept first proposed in the 1950s, researchers at the University of Michigan are using ORNL's Summit supercomputer to conduct trailblazing research that may finally unlock the engine's potential for ultrahigh-efficiency propulsion and power generation.

> "To me, Summit is a step change. Its compute power is something I did not expect. So we really had to increase our ambition once we got access to the machine. We changed our algorithmic frameworks, we changed our codes, we even changed how we answer the questions.
>
> — **Venkat Raman** professor of aerospace engineering, University of Michigan

UM professor of aerospace engineering Venkat Raman used Summit to execute combustion simulations with unprecedented fidelity and speed to help develop the rotating detonation engine, or RDE.

"To me, Summit is a step change. Its compute power is something I did not expect. So we really had to increase our ambition once we got access to the machine," Raman said. "We changed our algorithmic frameworks, we changed our codes, we even changed how we answer the questions."

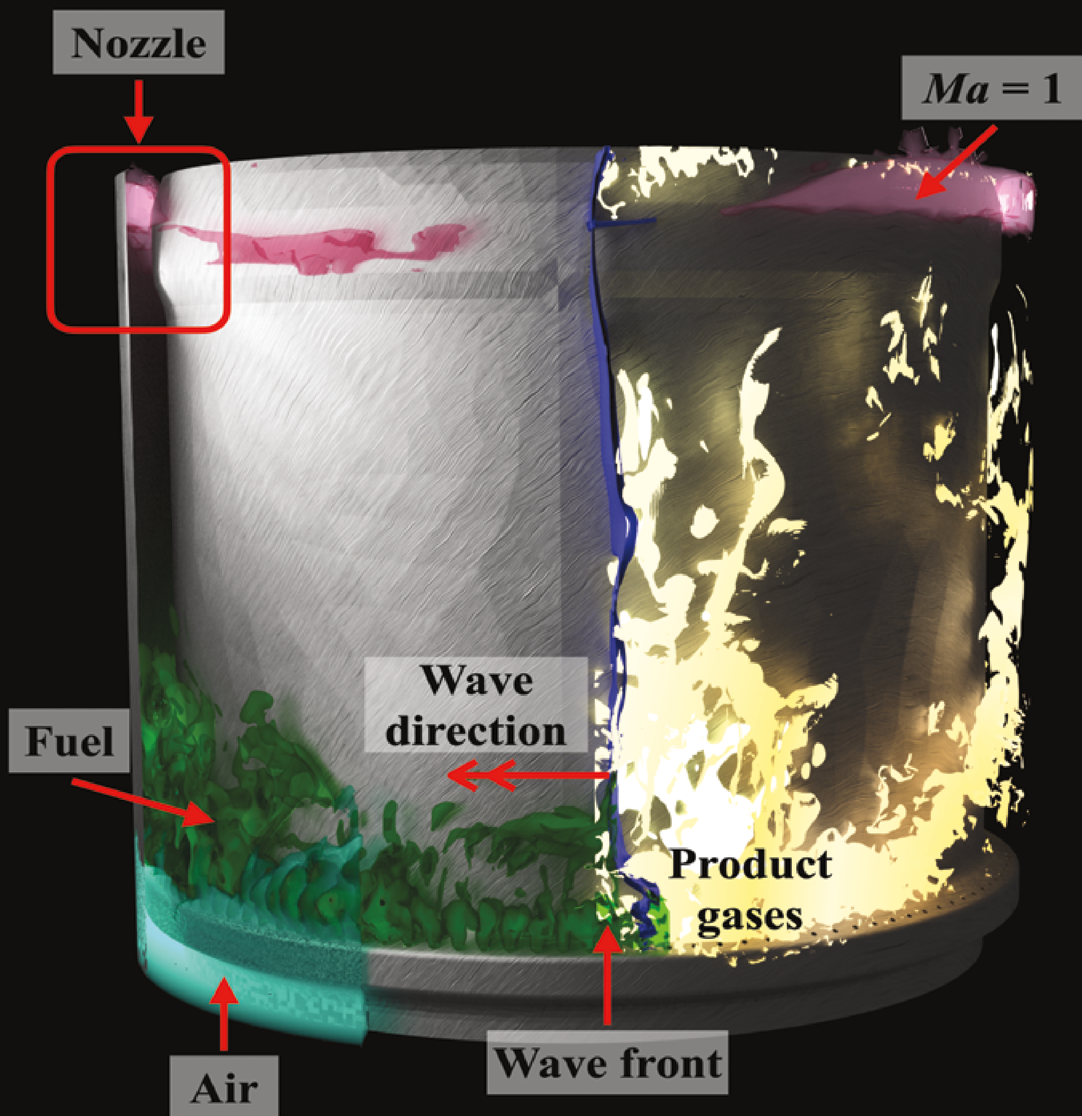
The concept for RDEs was pioneered in the 1950s by the late James Arthur Nicholls, a professor in UM's Department of Aeronautical (now Aerospace) Engineering. Like many innovations in engineering, his resulted from asking an unorthodox question. Noting how malfunctioning rocket engines tended to explode, it made him wonder: What if such explosions were used in an engine to propel rockets?

A conventional rocket engine uses compressors to send a pressurized mixture of fuel and oxygen into a combustor, where the mixture ignites and burns via deflagration — essentially the same combustion process used by car engines or jet turbines. This deflagration releases energy, which can be used to drive a mechanical device, such as a turbine, or to thrust a rocket upward.

An RDE, on the other hand, burns its fuel by detonation rather than deflagration; combustion occurs in a wave front that is led by a sustained shockwave that continuously rotates within a cylindrical combustor's inner and outer walls. The result is a much higher degree of efficiency in pulling energy out of the fuel, since the detonation wave, in effect, acts as its own compressor even as it's releasing energy.

"The application we're looking at here is in power generation with a 3 to 5 percentage-point improvement in overall cycle efficiency. This is huge in the gas turbine world, where they're usually looking at a tenth of a percent of improvement in efficiency. Ultimately, that boils down to lowering your energy bill," said Don Ferguson, a research engineer at the National Energy Technology Laboratory's Research & Innovation Center.

Understanding all of the physics at play during an RDE detonation wave is critical to making the technology safe for



A practical RDE configuration highlighting the detonation wave, the reactant fuel–air mixture and the product gases, with a nozzle choking the postdetonation exhaust flow. Image courtesy University of Michigan

commercial use. For example, in order to replace an aircraft engine with a detonation engine, you must take into account all of the plane's different operating conditions — taxiing, taking off, cruising — to ensure the detonation engine's efficiency remains stable. The first step is to understand what happens to the key physics inside the engine when those conditions change.

"So many of the techniques we have for conventional jet engines and gas turbines don't work in these kinds of extreme environments. So simulations are the only way to go," Raman said. "However, simulating the complicated physics in RDEs is very challenging. These simulations have as much physics as the most complicated problem you can think of — fluid mechanics, shockwaves, chemical reactions, a heat transfer to the wall."

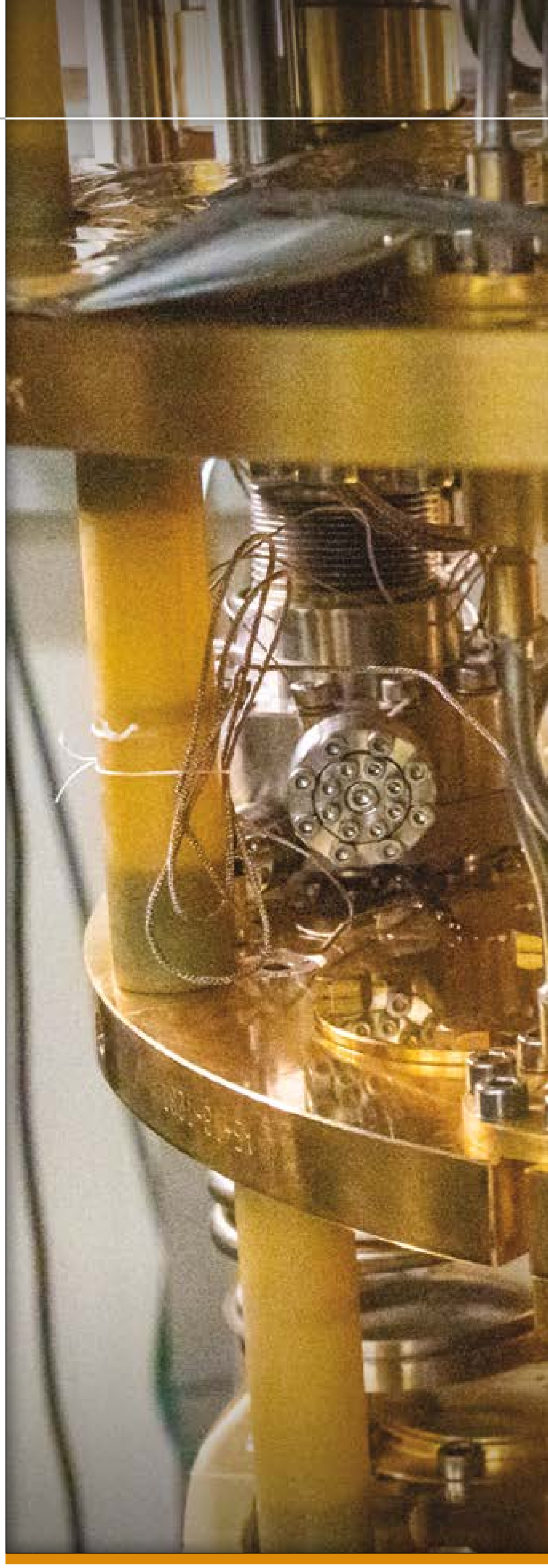
At first, Raman and his team of graduate students got off to a slow start, putting only about 30 percent of their simulations code — based on the open-source modeling software OpenFOAM — onto Summit's graphics processing units. This approach did not result in much of a speedup. But, with guidance from Oak Ridge Leadership Computing Facility staff, the students completely rewrote Open-FOAM to take full advantage of Summit's GPU-powered architecture, and now 95 percent of the code runs on GPUs.

Furthermore, the team recognized the opportunity to leverage the advantages GPUs have for artificial intelligence algorithms and consequently trained neural networks to speed up the modeling program even further — a first in the field.

"This allows us to get, in some extreme cases, about 1,000-times-faster simulations compared to if you just did conventional calculations," Raman said. "More than even speedup, you can also answer different questions. It's not an incremental change."

ORNL, partners

receive $115 million to establish Quantum Science Center



by Scott Jones
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From computers exponentially more powerful than today's leading systems to sensors with unprecedented precision, quantum technologies promise to greatly increase our understanding of the world and, by extension, fundamentally transform it.

In recognition of this potential, DOE has selected ORNL to lead a collaboration charged with developing quantum technologies that will usher in a new era of innovation.

The Quantum Science Center, one of five newly formed quantum research centers established by DOE, will receive $115 million over five years from the Office of Science to explore the ability of topological quantum materials to manipulate, transfer and store quantum information. The center will transition this knowledge to the private sector for use in practical applications.

The center supports the National Quantum Initiative Act of 2018 by enhancing America's national security and retaining its global leadership in scientific research and development — goals that require broad expertise and capabilities.

"We pulled together a fantastic team from four national laboratories, three industry partners and nine universities to overcome key roadblocks in quantum state resilience, controllability and ultimately scalability of quantum technologies," QSC Director and ORNL physicist David Dean said. "We are prepared to catalyze quantum materials, computing and devices research to significantly impact the national quantum ecosystem."

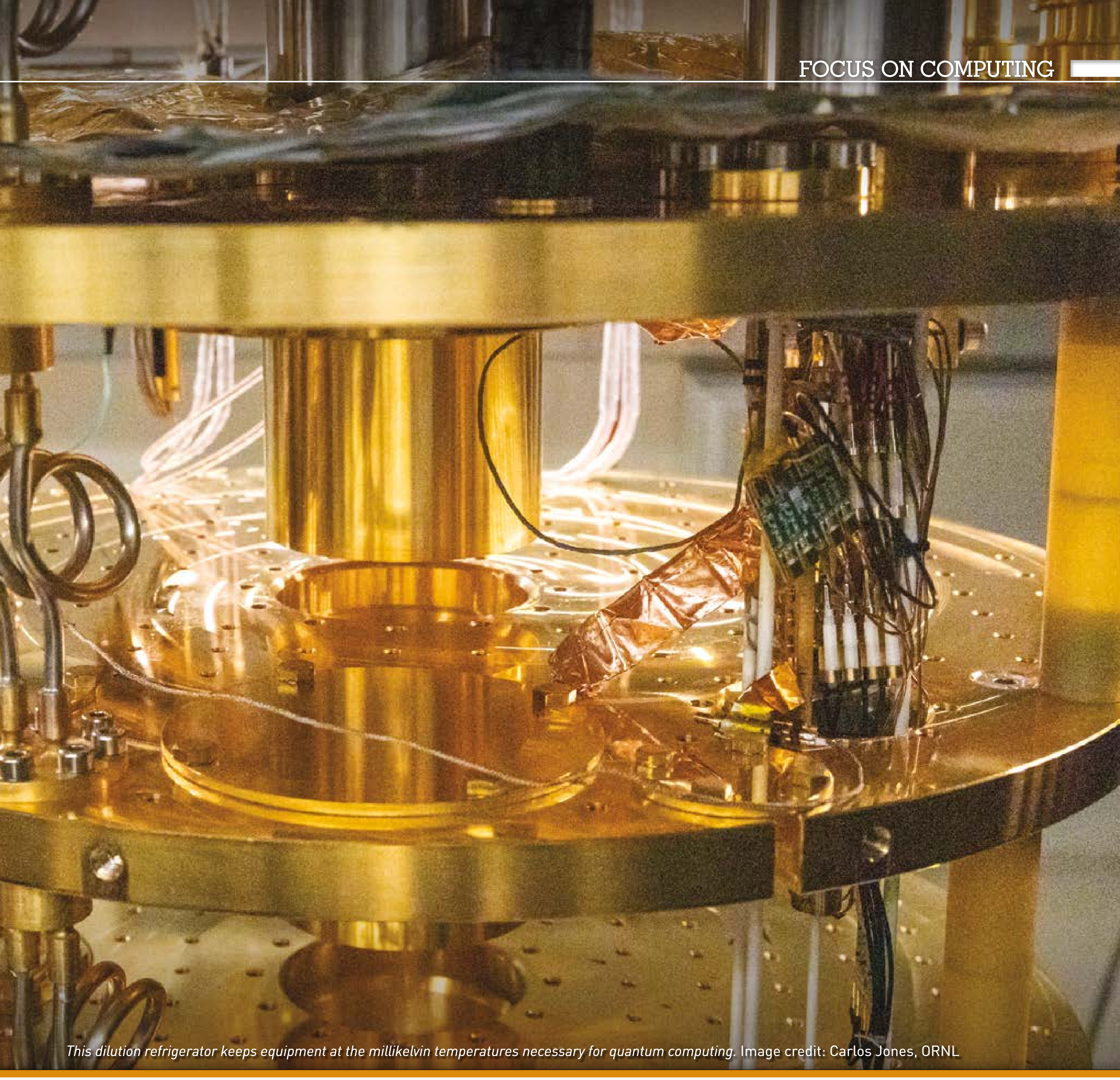
The QSC's research goals are organized around three scientific focus areas:

- Quantum materials discovery and design, for which QSC researchers will investigate and exploit the novel properties of topological materials for computing.
- Quantum algorithms and simulations, for which QSC researchers will develop and test algorithms for quantum computers and sensors.
- Quantum devices and sensors for discovery science, for which QSC researchers will co-design new quantum devices and sensors with unprecedented performance for real-world applications in the DOE domain.

This co-design philosophy is at the heart of the QSC's research model. By engaging stakeholders from its inception, the center will ensure resulting advances meet the needs of the private sector and American research communities.

"Our scientific goals rely on a co-design process to maximize the impact and readiness of new quantum devices, quantum simulations and quantum sensors within the next five years," said Travis Humble, QSC deputy director and head of the Oak Ridge Leadership Computing Facility's Quantum User Program. "We have prioritized engagement with U.S. industry to identify near-term opportunities to develop quantum technologies that will ensure long-term economic competitiveness."

Also integral to the QSC's mission is the development of the next generation of scientists and engineers. By engaging students and postdoctoral associates in



This dilution refrigerator keeps equipment at the millikelvin temperatures necessary for quantum computing. Image credit: Carlos Jones, ORNL

research activities at partnering institutions, the center will offer a rich environment for cultivating the expertise necessary to ensure America leads the quantum revolution.

As headquarters for the QSC, ORNL will leverage its quantum research program, which dates back nearly two decades, and the expertise of 25 staff members dedicated to advancing the state of the art in quantum information science. The laboratory set the record for quantum information transfer in 2017 and partnered with industry to demonstrate quantum supremacy — the notion that a quantum computer could outperform a classical computer — in October 2019.

"Our goal is to build a research team representing diverse scientific and engineering disciplines and to focus their capabilities on advances in materials, computing and technology development," ORNL Director Thomas Zacharia said. "We are honored by this award and look forward to the Quantum Science Center's contributions to U.S. economic competitiveness, national security and scientific leadership."

Partner organizations include Caltech, ColdQuanta, Fermilab, Harvard University, IBM, Los Alamos National Laboratory, Microsoft, Pacific Northwest National Laboratory, Princeton University, Purdue University, the University of California at Berkeley; the University of California at Santa Barbara, the University of Maryland, the University of Tennessee at Knoxville, and the University of Washington.

Process for 'Two-faced' nanomaterials may aid energy, information tech

by Dawn Levy
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An ORNL-led team has used a simple process to implant atoms precisely into the top layers of ultra-thin crystals, yielding two-sided structures with different chemical compositions. The resulting materials, known as Janus structures after the two-faced Roman god, may prove useful in developing energy and information technologies.

"We're displacing and replacing only the topmost atoms in a layer that is only three atoms thick, and when we're done, we have a beautiful Janus monolayer where all the atoms in the top are selenium, with tungsten in the middle and sulfur in the bottom," said David Geohegan, who leads ORNL's Functional Hybrid Nanomaterials Group. "This is the first time that Janus 2D crystals have been fabricated by such a simple process."

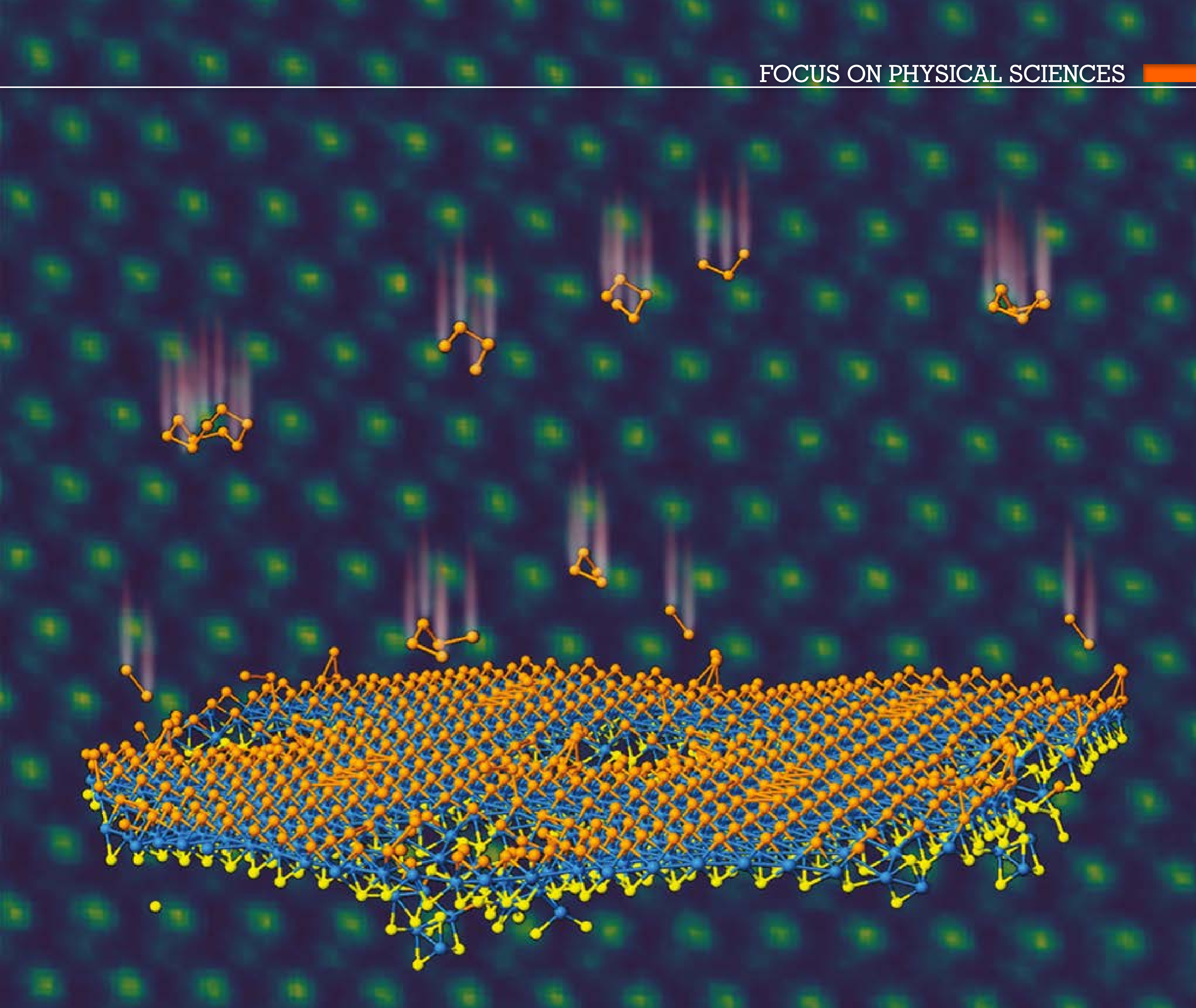
Because Janus monolayers have a built-in electric field that allows them to separate charge, they are interesting materials for applications ranging from photovoltaics to quantum information. Yu-Chuan Lin, a former ORNL postdoctoral fellow who led the study, added, "With this straightforward technique, we can put different atoms on the top or bottom of different layers to explore a variety of other two-faced structures."

This study probed 2D materials called transition metal dichalcogenides, or TMDs, which are valued for their electrical, optical and mechanical properties. Tuning their compositions may improve their abilities to separate charge, catalyze chemical reactions or convert mechanical energy to electrical energy and vice versa.

A Janus monolayer has different atoms on top and bottom, like the sandwich cookie at right held by materials scientist Yu-Chuan Lin. Image credit: Christopher Rouleau, ORNL

A single TMD layer is made of a layer of transition metal atoms, such as tungsten or molybdenum, sandwiched between layers of chalcogen atoms, such as sulfur or selenium. A molybdenum disulfide monolayer, for example, features molybdenum atoms between layers of sulfur atoms, structurally similar to a sandwich cookie with a creamy center between two chocolate wafers. Replacing one side's sulfur atoms with selenium atoms produces a Janus monolayer, akin to swapping one of the chocolate wafers with a vanilla one.

The method uses a pulsed laser to vaporize a selenium target into a hot plasma of clusters of two to nine selenium atoms. This plasma beam is directed to strike pregrown tungsten disulfide monolayer crystals.



Selenium atoms (orange) implant in a monolayer of blue tungsten and yellow sulfur to form a Janus layer. In the background, electron microscopy confirms atomic positions. Image credit: Yu-Chuan Lin, ORNL

The key to success is bombarding the crystals with clusters having a precise amount of energy. Throw a bullet at a door, for example, and it bounces off the surface. But shoot the bullet at the door, and the bullet rips right through. Implanting selenium clusters into just the top of the monolayer is like shooting a door and having the bullet stop in its surface.

To controllably slow the selenium clusters, the researchers added argon gas in a pressure-controlled chamber. Limiting the kinetic energy restricts the penetration of atomically thin layers to specific depths. Injecting a pulse of atom clusters at low energy temporarily crowds and displaces atoms in a region, causing local defects and disorder in the crystal lattice. "The crystal then ejects the extra atoms to heal itself and recrystallizes into an orderly lattice," Geohegan explained.

To prove that they had achieved a Janus structure, researchers used many techniques. For example, Chenze Liu and Gerd Duscher, both of the University of Tennessee, Knoxville, and Matthew Chisholm of ORNL used high-resolution electron microscopy to examine a tilted crystal to identify which atoms were in the top layer (selenium) versus the bottom layer (sulfur).

ORNL's Mina Yoon used supercomputers at the Oak Ridge Leadership Computing Facility to calculate the energy dynamics of replacing sulfur atoms with larger selenium atoms.

With molecular dynamics simulations, ORNL's Eva Zarkadoula showed clusters of selenium atoms colliding with the monolayer at different energies and bouncing off it, crashing through it or implanting in it — consistent with the experimental results.

Carbon-loving materials

target industrial emissions

by Ashley Huff
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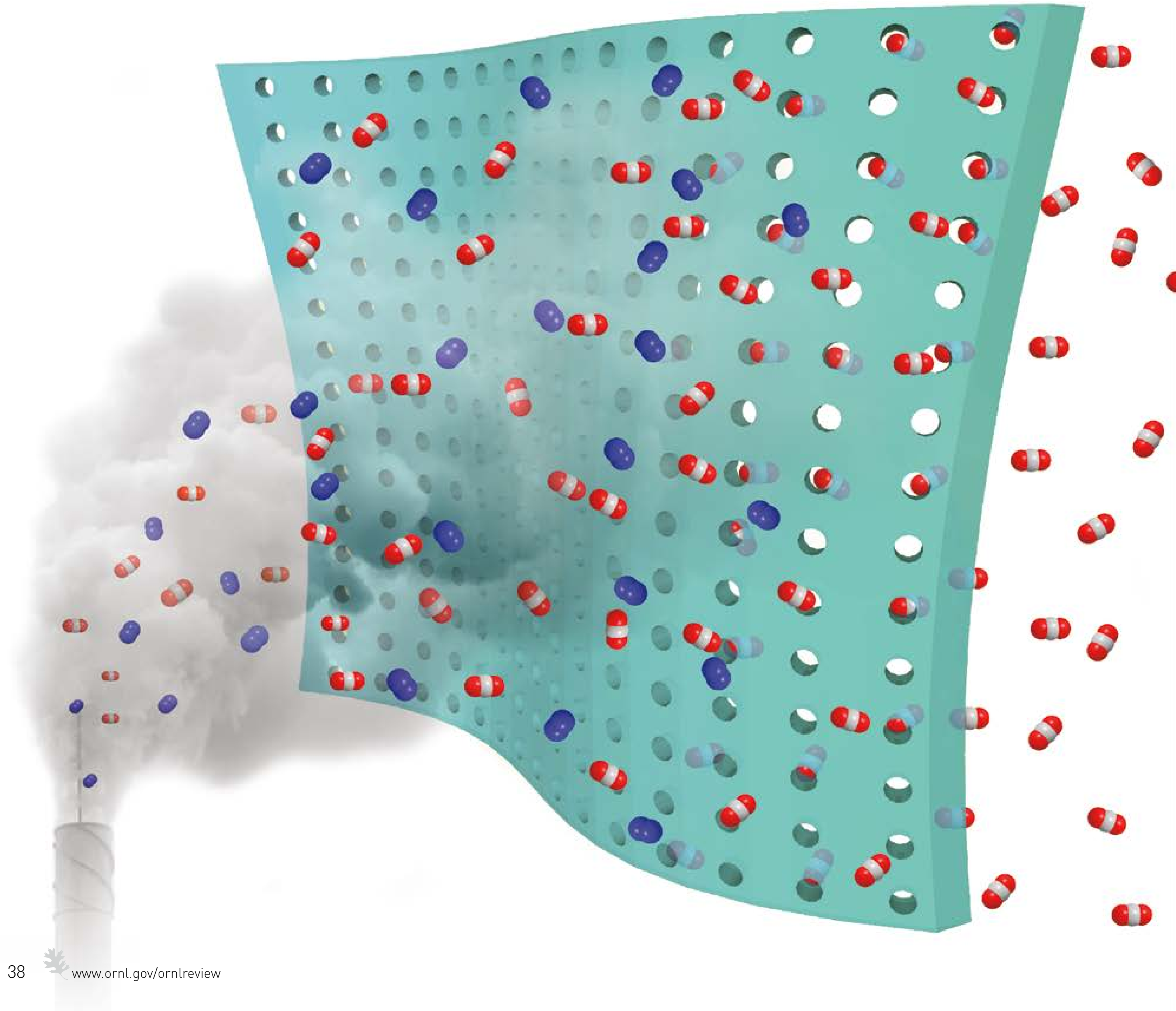

New carbon-loving materials may expand affordable options for reducing postcombustion emissions produced by fossil-fueled industries.

Researchers at ORNL and the University of Tennessee have showcased gas membrane materials that incorporate fluorine, demonstrating both performance boosts and lower-cost fabrication critical to scaling up the technology for industrial use.

Gas membranes are a promising carbon-capture technology. The concept is simple: A thin, porous membrane acts as a filter for exhaust gas, selectively allowing carbon dioxide to flow through freely into a collector that is kept under reduced pressure, but preventing oxygen, nitrogen and other gases from tagging along.

Unlike existing chemical methods to capture CO_2 from industrial processes, membranes are easy to install and can operate unattended for long periods with no additional steps or added energy costs. The catch is that new, cost-effective materials are needed to overcome performance bottlenecks and open practical pathways for commercial adoption.

Selectivity and permeability — rates measuring how effective and efficient materials are at targeting and sorting out CO_2 — are the key performance variables. That's because gas membranes need pressure on one side and, typically, a vacuum on the other to maintain a free-flow environment.

"Underperforming materials require more energy to push gases through the system, so advanced materials are key to keeping energy costs low," said ORNL's Ilja Popovs.

"Often there is a trade-off in how selective or how permeable you can make membranes that filter out carbon dioxide without allowing other gases to pass through. The ideal scenario is to create materials with high permeability and selectivity," said UT's Zhenzhen Yang.

No natural materials and only a few synthetic ones have exceeded what is called the Robeson upper limit, a boundary that constrains how selective and permeable most materials can be before these rates start to drop.

Materials with sufficiently high selectivity and permeability for efficient gas separation are rare and often made from expensive starting materials whose production requires either long and tedious synthesis or costly transition metal catalysts.

"Our first step was to create a unique fluorine-based polymer using simple chemical methods and commercially available starting materials," Yang said.

Next, researchers transformed, or carbonized, the material using heat to give it the porous structure and functionality needed for capturing CO_2. The two-step process preserved the fluorinated groups and boosted CO_2 selectivity in the final material, overcoming a fundamental hurdle encountered in other synthetic methods.

"The approach resulted in a carbon dioxide–philic material with high surface area and ultra-micropores that is stable in high-temperature operating conditions," Yang said. "All of these factors make it a promising candidate for carbon-capture and separation membranes."

> *"Our success was a material achievement that demonstrates feasible routes for leveraging fluorine in future membrane materials. Moreover, we achieved this goal using commercially available, inexpensive starting materials.*
>
> — ORNL organic chemist **Ilja Popovs**

Researchers set out to test a hypothesis that introducing fluorine atoms into membrane materials could help address these challenges.

Fluorine, used to make consumer products such as Teflon and toothpaste, offers CO_2-attracting properties that make it promising for carbon-capture applications. It is also widely available, making it a relatively affordable option for low-cost fabrication methods. Research on fluorinated gas membranes has been limited because of fundamental challenges associated with incorporating fluorine into materials to realize its carbon-loving functionality.

The material's novel design contributes to its exceptional performance, observed in high selectivity and permeability rates that exceed the Robeson upper limit, something only a handful of materials have accomplished.

"Our success was a material achievement that demonstrates feasible routes for leveraging fluorine in future membrane materials. Moreover, we achieved this goal using commercially available, inexpensive starting materials," Popovs said.

This basic discovery expands the limited library of practical options for carbon-capture membranes and opens new directions for developing fluorinated membranes with other task-specific functionalities.

Researchers at ORNL and the University of Tennessee have demonstrated a novel fabrication method for affordable gas membranes that can remove carbon dioxide from industrial emissions. Image credit: Zhenzhen Yang, University of Tennessee

Summit simulations uncover COVID-19 connections

by Elizabeth Rosenthal
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Using artificial intelligence techniques and ORNL's Summit supercomputer, researchers from ORNL and Georgia Tech have analyzed millions of COVID-19–related scientific papers to identify previously unknown connections among seemingly disparate biomedical topics and compile them into a publicly available dataset.

Insights gleaned from these connections could help scientists and medical professionals identify effective drugs, develop new vaccines and discover other potential COVID-19 cures.

These analyses involved sifting at unprecedented speeds through the PubMed database maintained by the National Library of Medicine, as well as the COVID-19 Open Research Dataset, or CORD-19. Examining a subset of 6 million medical documents published between 2010 and 2015 took 80 minutes, less time than it takes to play a standard game of soccer.

Using their method, the team — ORNL's Ramki Kannan, Piyush Sao, Hao Lu and Robert Patton and Georgia Tech's Vijay Thakkar and Rich Vuduc — estimates that completing similar calculations to extract information from a total of 18 million documents published over decades will take less than a day.

"The variations in COVID-19 symptoms and treatment responses seen around the world demand a better method of rapid clinical and scientific evaluation," Kannan said. "Simultaneously comparing countless genotypic, phenotypic and therapeutic models is extremely difficult, and the risk of leaving any stone unturned is much higher during the pandemic."

> *"It's impossible to manually connect results from such a vast number of studies to find possible COVID-19 cures, so we need to extract relevant concepts from these biomedical studies and identify the best research directions to pursue, which requires a major breakthrough in path prediction over a massive knowledge graph.*
>
> — ORNL Data and AI Systems Research Section Head **Thomas Potok**

To trace these direct and indirect connections, the researchers studied the simulation results in conjunction with keywords related to severe acute respiratory syndrome coronavirus 2, or SARS-COV-2, the novel coronavirus that infects host cells with the COVID-19 disease.

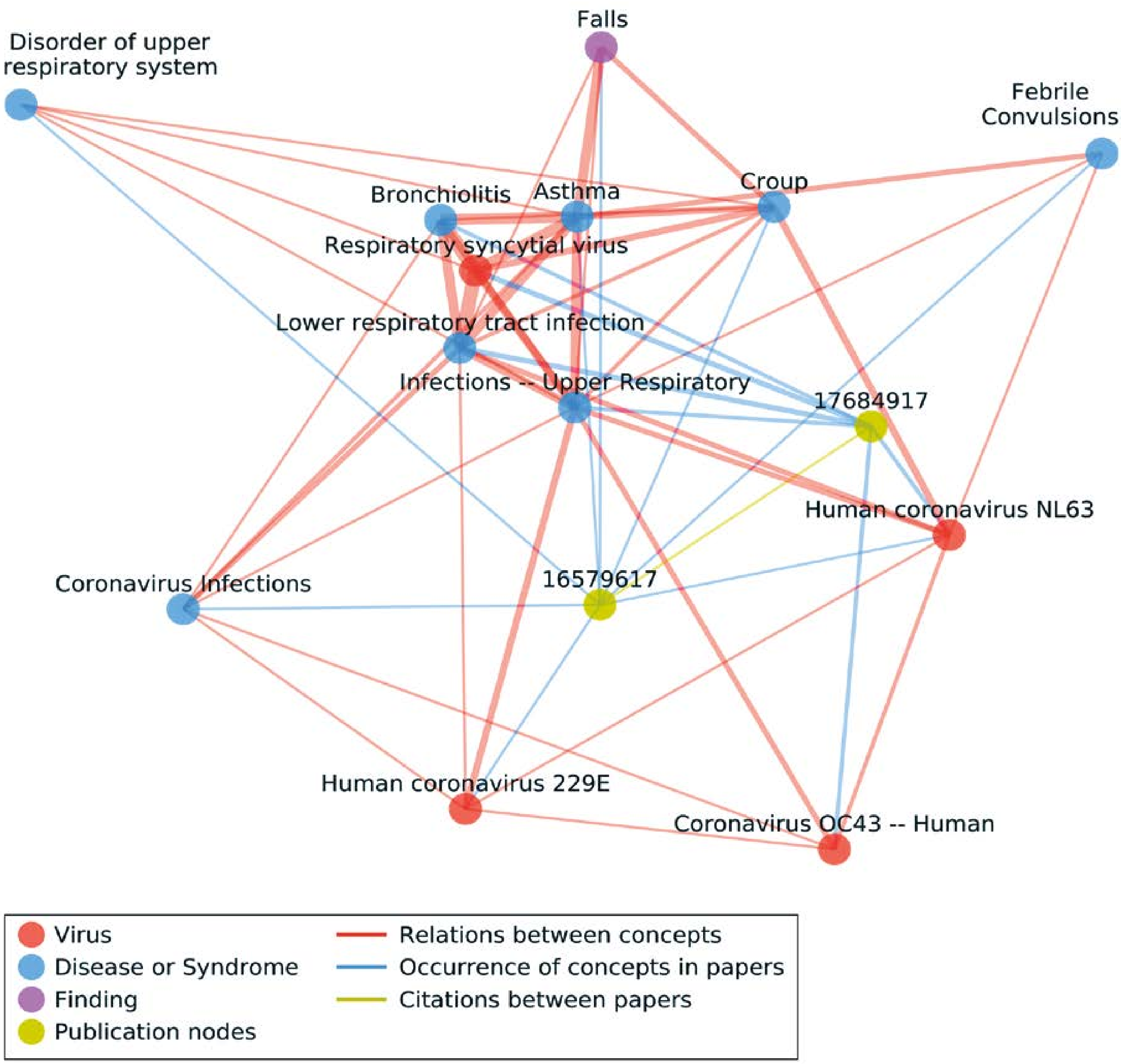
Notably, they found relationships between COVID-19 symptoms and existing treatments for other medical conditions that experts could exploit not only to treat individual patients but also to slow or stop the spread of the virus worldwide.

"It's impossible to manually connect results from such a vast number of studies to find possible COVID-19 cures, so we need to extract relevant concepts from these biomedical studies and identify the best research directions to pursue, which requires a major breakthrough in path prediction over a massive knowledge graph," said ORNL's Thomas Potok, Data and AI Systems Research section head, who advises the team.

To enable such a large-scale investigation, the team developed a state-of-the-art GPU-accelerated high-performance computing algorithm called the Distributed Accelerated Semiring All-Pairs Shortest Path, or DSNAPSHOT.

This new algorithm achieved more efficient and accurate sustained performance than comparable tools, an accomplishment that made the team a finalist for the Association for Computing Machinery's annual Gordon Bell Prize. DSNAPSHOT can be applied to medical databases beyond CORD-19 and PubMed, and the researchers have tested their algorithm on 12 other text, gene, network and scientific datasets.

"It's beautiful to see the way that decades of lessons learned on classical



The ORNL–Georgia Tech team's knowledge graph illustrates the potentially life-saving links between COVID-19 symptoms and existing drug therapies approved by the U.S. Food and Drug Administration. Image credit: Dasha Herrmannova, ORNL

problems in high-performance computing translate into new domains," Vuduc said.

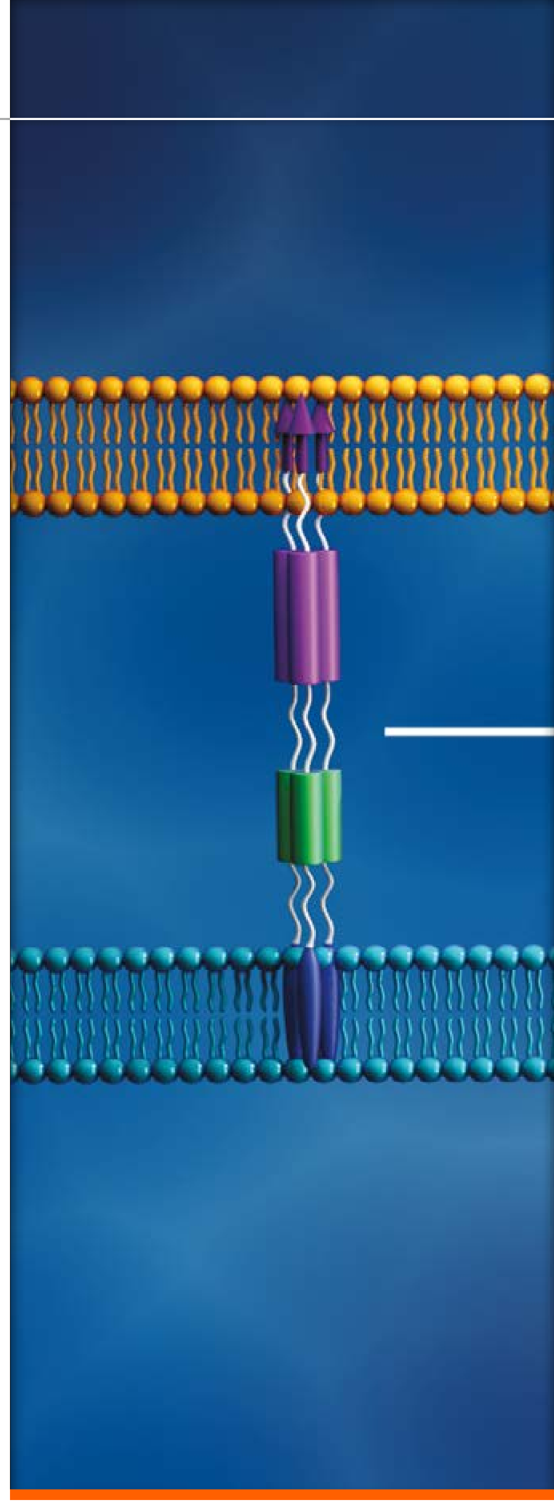
The researchers plan to continue mapping connections among biomedical concepts to keep up with the latest COVID-19 findings. Kannan anticipates that integrating this knowledge into machine learning algorithms and other AI workflows at a global scale could facilitate better data mining and knowledge sharing processes as the scientific community races to end the pandemic.

"The world's response to different COVID-19 clinical presentations and treatment responses, as well as its preparation for future pandemics, would improve with the ability to cross reference scientific literature to continuously search for underlying correlations," he said. "These connections could be exploited to treat millions of COVID-19 patients and may also prepare us to fight other diseases going forward."

This work was funded by DOE's Advanced Scientific Computing Research program.

Neutrons probe cellular invasion processes of

COVID-19 infections



by Olivia Trani and Paul Boisvert
tranior@ornl.gov

ORNL researchers are using neutrons to better understand how SARS-CoV-2, the coronavirus responsible for COVID-19 disease, infects human cells at the molecular level. In doing so, they hope to help experts discover ways to slow or stop the virus from spreading.

Neutrons are capable of probing biological materials in a wet environment without damaging them, allowing researchers to study the infection processes at their earliest stages.

Some researchers are focusing on studying SARS-CoV-2 spike proteins, barb-like structural proteins on the virus's surface that trigger the infection process. Others are studying envelope proteins, called E-proteins, which subsequently invade the cell's manufacturing centers to enable the virus's genetic material to make copies of itself and assemble new viruses.

When SARS-CoV-2 encounters a potential host cell, its spike protein splits into two subunits, S1 and S2. The S1 subunit latches onto the cell, causing the S2 subunit to activate and help the virus and cell membranes fuse. The E-proteins can then enter the cell and begin their work.

This type of cellular invasion is typical of viral infections, from a common cold to a seasonal flu. However, the E-proteins of SARS-CoV-2 have an ion channel that increases the permeability of the host cell membrane and triggers inflammation. The result can be a significant fluid buildup in the lungs and, in some people, swelling in other body tissues. This can turn what might otherwise resemble a cold or the flu into acute respiratory distress syndrome, which can cause breathing problems and multiple organ failure.

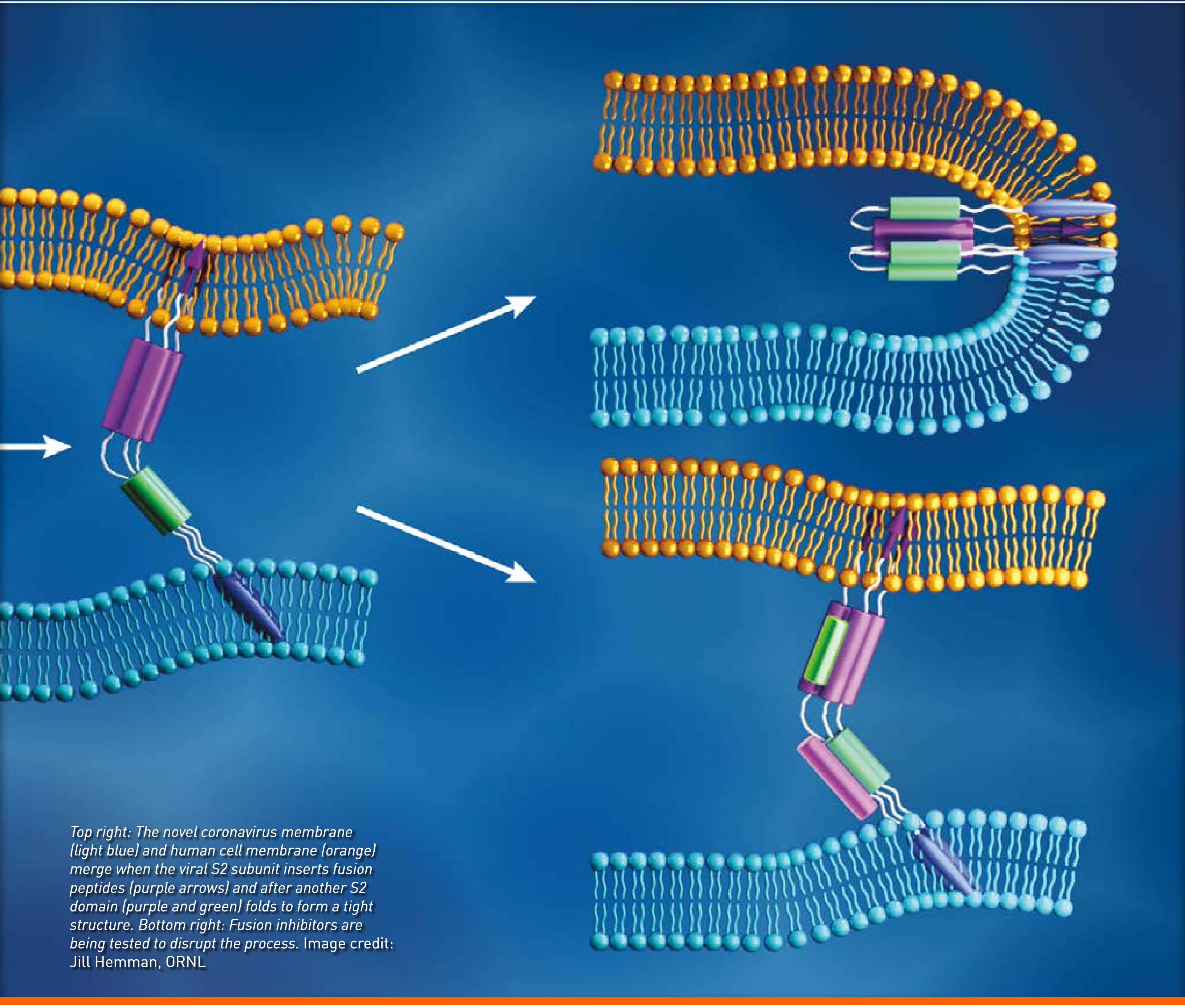
Focus on longest-lasting treatments

The scientists are focusing on the S2 subunit and E-protein because they mutate less often than other features, so treatments inhibiting them may stay effective longer. E-proteins are promising targets also because of their ion channel.

"In laboratories, ion channel blockers have proven effective in limiting inflammation caused by a similar coronavirus, SARS-CoV, which caused a deadly pandemic in 2002," said Jesse Labbé, a cellular and molecular fungal geneticist in ORNL's Biosciences Division.

To better understand the dynamics of the virus and host cell membranes, the researchers are employing the liquids reflectometer neutron instrument at ORNL's Spallation Neutron Source.

"At ORNL, we have the right tools to study the dynamics of biological interactions under physiological conditions, as



Top right: The novel coronavirus membrane (light blue) and human cell membrane (orange) merge when the viral S2 subunit inserts fusion peptides (purple arrows) and after another S2 domain (purple and green) folds to form a tight structure. Bottom right: Fusion inhibitors are being tested to disrupt the process. Image credit: Jill Hemman, ORNL

opposed to crystallized samples. This allows us to better understand how the S2 subunit and E-protein act naturally in a wet environment," said Minh Phan, postdoctoral research associate and principal investigator for some of the S2 and E-protein experiments.

Collaboration is key

Of course, learning more about the S2 subunit and its behaviors depends on the ability to grow quality samples, which includes synthesizing lipid bilayers to serve as membrane models and preparing them for experimentation.

"This virus is extremely delicate in its components, and it's a big challenge to get these materials to the neutron instrument," said John Ankner, an instrument scientist on the projects. "That's why involving other ORNL labs and the University of Tennessee was so crucial. Each step that helps get the sample onto our instrument requires the expertise of many people."

Labbé, Phan and Ankner all noted that much of their research was possible only through collaborations with other labs at ORNL and with outside institutions.

The information derived from these experiments will help steer the teams' next efforts in selecting and testing drug candidates, such as fusion inhibitors that successfully blocked original SARS-CoV infections. The data obtained from these experiments could also inform other studies focused on developing therapeutics and vaccines.

Advanced manufacturing, carbon fiber research help fight COVID-19

by Jennifer Burke
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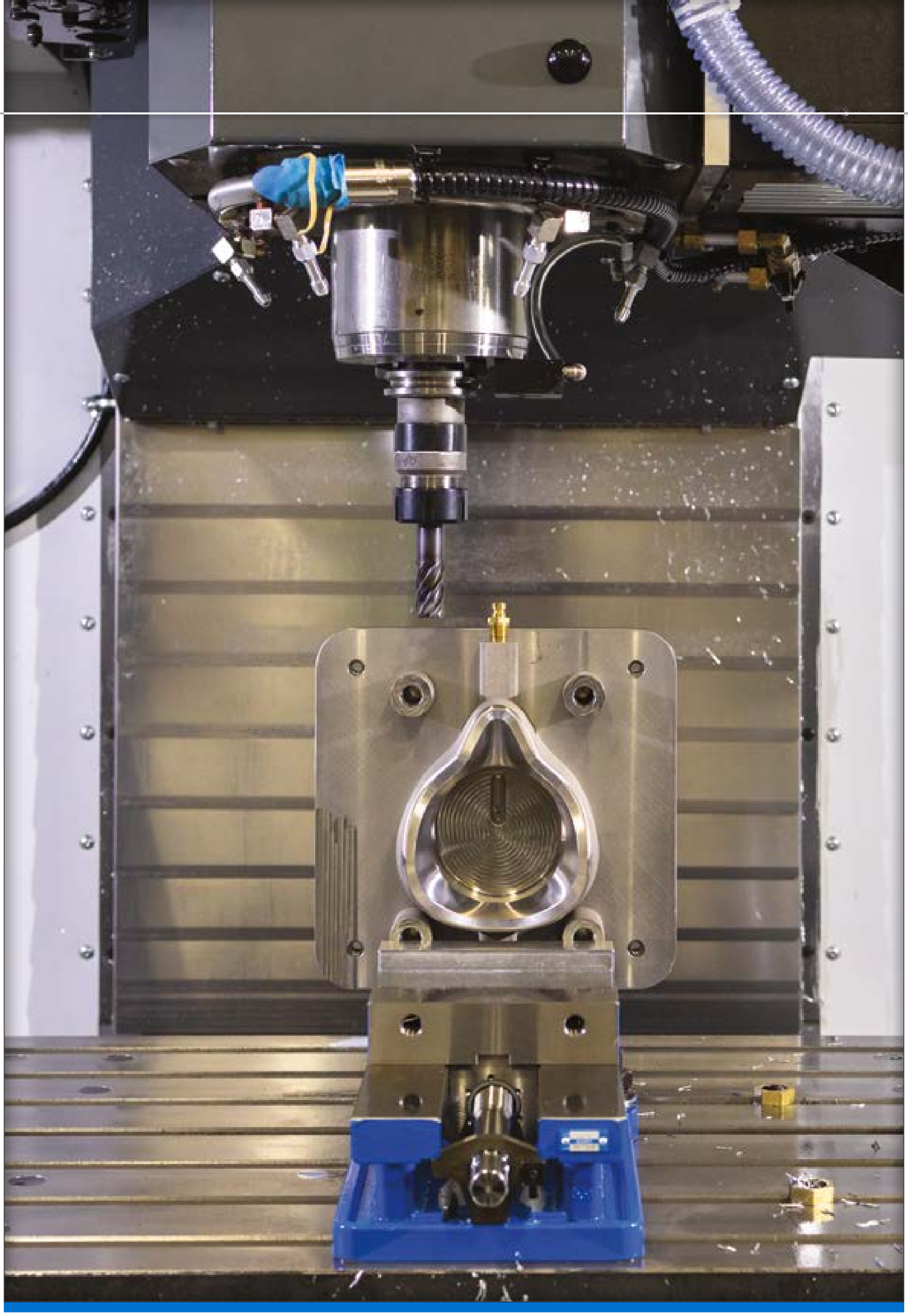
In the fight against COVID-19, ORNL researchers at DOE's Manufacturing Demonstration and Carbon Fiber Technology facilities have used materials science and additive manufacturing to enable U.S. industry to mass-produce face masks and shields for health care workers.

Working with partners from the Department of Defense Industrial Base Analysis and Sustainment Program and the Department of Health and Human Services, ORNL researchers developed tooling to create molds for face masks and shields. These efforts are part of a collaboration between DOE and DOD called the America's Cutting Edge program, a national initiative for machine tools technology development and advancement.

Health care workers depend on face shields to protect them from infectious diseases. A method commonly used to manufacture the shields is injection molding, which works by filling a metal mold with molten plastics to produce large volumes of shields. Face shields can be 3D-printed, but the only way to produce them rapidly is through injection molding.

Researchers at DOE's Carbon Fiber Technology Facility used melt-blowing technology to produce the filter material that lines N95 face masks and protects health care workers in the fight against COVID-19. Image credit: Carlos Jones, ORNL



ORNL researchers at DOE's Manufacturing Demonstration Facility developed the tooling for a prototype reusable mask, enabling industry to rapidly produce up to 300,000 masks per week.
Image credit: Carlos Jones, ORNL

> *"To do injection molding, you need tooling. We've created tools in days instead of months. Our efforts made it possible for industry to scale up production.*
>
> — ORNL COVID-19 manufacturing lead researcher **Lonnie Love**

"To do injection molding, you need tooling," said ORNL's Lonnie Love, lead researcher on ORNL's COVID-19 manufacturing efforts. "We've created tools in days instead of months. Our efforts made it possible for industry to scale up production."

At the MDF, researchers worked with Uday Vaidya, ORNL/University of Tennessee Governor's Chair in Advanced Composites Manufacturing, to design a mold for making the plastic band that fits to the head and holds the shield in place. ORNL's research team then 3D-printed and machined a mold ready for industry use within three days.

In addition to face shields, ORNL developed and designed the tooling for a reusable face mask prototype. The mask is made of five parts: a retention ring band, a hard outer shell, filter material, a softer inner shell and an inner retention ring. Rectangular holes can be drilled into the outer mask to add straps.

"With five sets of tools, industry can potentially make 300,000 reusable masks per week," Love said.

At the CFTF, researchers were presented with the challenge of producing filtration material for masks on existing equipment typically used to mass-produce precursor material for carbon fiber production.

CFTF Director Merlin Theodore turned to the precursor line's melt-blowing capability for the answer. The material, called N95, is made of two plies of melt-blown polypropylene, a nonwoven material that is permanently electrostatically charged with millions of microfibers layered on top of each other. The filter is capable of removing more than 95 percent of submicron particles found in viruses. Melt blowing is a nonwoven process that makes microfibers into a fabric by scattering a polymer resin at a high air velocity. Randomly deposited fibers form a sheet of material applicable for filtration.

Theodore and her team worked with Peter Tsai, a retired University of Tennessee professor and N95 material inventor, to develop an inline electrostatic charging technology for the melt-blowing line.

Researchers across multiple disciplines in materials science, characterization and systems, and electrical engineering collaborated to adjust the speed and feed of the material to achieve optimum production targets. The electrostatic charging device was then machine-tooled and built by researchers at the MDF and finally transferred to industry for the mass production of N95 material.

"Our COVID-19 research is a great example of why national labs and DOE's user facilities exist. We're here to serve the nation, to find solutions and to deliver technology for the betterment of the U.S.," Love said.

Celebrating the next generation of great scientists

by Karen Dunlap
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Scientists often do their most formative work at the beginning of their careers, which is one reason DOE's Office of Science picks exceptional researchers to receive significant funding through its Early Career Research Program.

This year, three ORNL scientists made the list and will receive grants for $500,000 per year for five years to cover salary and research expenses.

> *"These early career researchers demonstrate the breadth of scientific inquiry at Oak Ridge. They are investigating complex subjects with global impact, including comprehensive climate modeling, the search for new physics and efficient fusion energy. I look forward to seeing what these talented young scientists accomplish.*
>
> — ORNL Director **Thomas Zacharia**

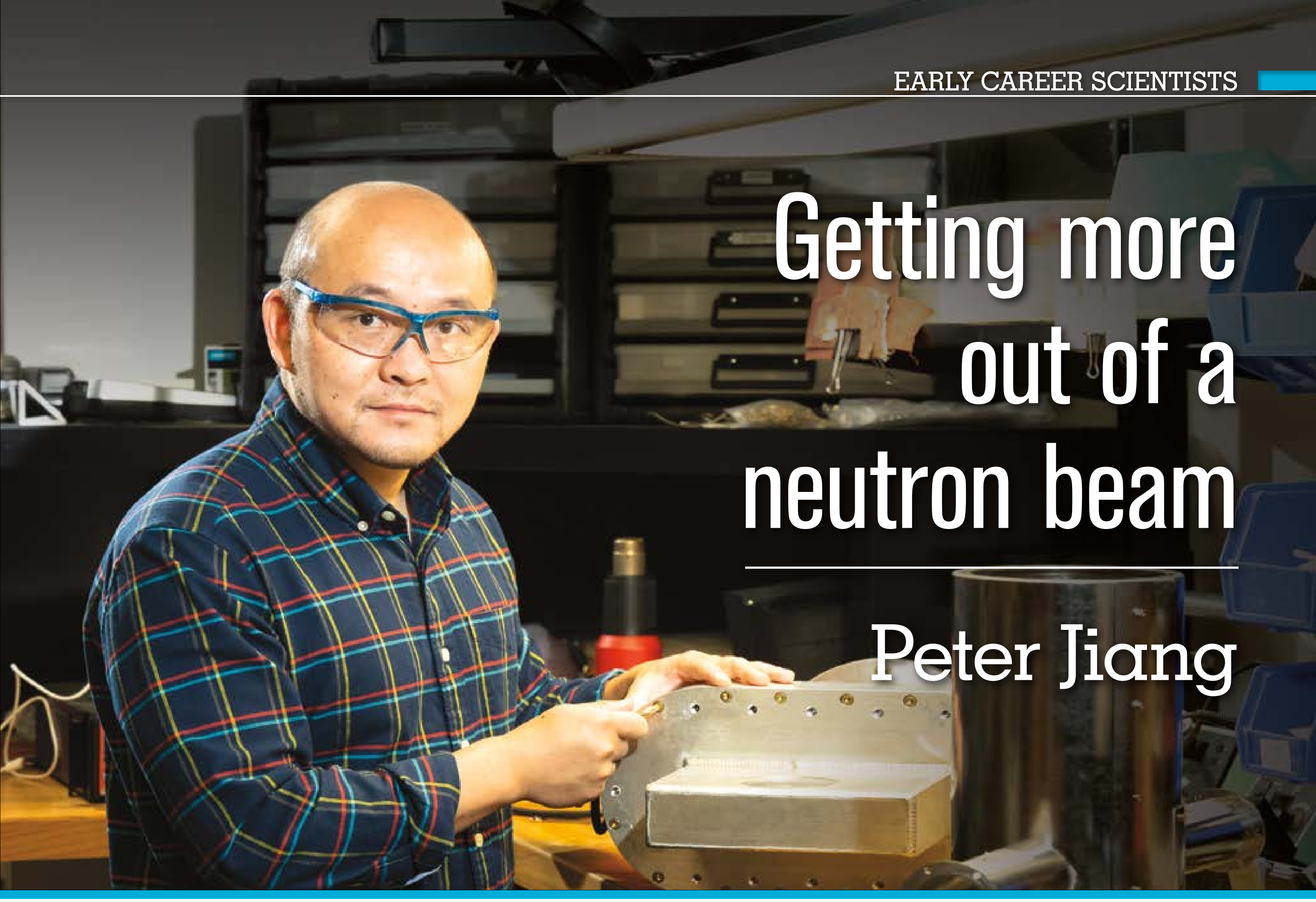
"These early career researchers demonstrate the breadth of scientific inquiry at Oak Ridge," ORNL Director Thomas Zacharia said. "They are investigating complex subjects with global impact, including comprehensive climate modeling, the search for new physics and efficient fusion energy. I look forward to seeing what these talented young scientists accomplish."

The ORNL researchers receiving awards are:

- Peter Jiang, a polarization scientist in the Neutron Technologies Division, who was selected by the Basic Energy Sciences program for his proposal, "Realization of Full Neutron Polarization Control: Next Generation Spherical Neutron Polarimetry for Neutron Scattering."
- Elijah Martin, a scientist in the Fusion Energy Division, who was selected by the Fusion Energy Sciences program for his proposal, "Investigation of Helicon and Lower Hybrid Wave Coupling with the Edge Plasma for Current Drive Optimization in the Tokamak Using Laser Spectroscopy."
- Benjamin Sulman, a scientist in the Environmental Sciences Division, who was selected by the Biological and Environmental Research program for his proposal, "Simulating Estuarine Wetland Function: Nitrogen Removal, Carbon Sequestration, and Greenhouse Gas Fluxes at the River-Land-Ocean Interface."

"The Department of Energy is proud to support funding that will sustain America's scientific workforce and create opportunities for our researchers to remain competitive on the world stage. By bolstering our commitment to the scientific community, we invest in our nation's next generation of innovators," DOE said in a statement.

Read on to learn more about the three scientists whose proposals were funded.



Getting more out of a neutron beam

Peter Jiang

by Karen Dunlap
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Peter Jiang has been captivated by physics since his childhood in China.

"I've always been interested in physical phenomena. Why is there a rainbow out there? Why does it have different colors? What makes the waves in the pond? When you throw a stone in the pond, why do the waves fluctuate up and down?" Jiang said. "All those small things got me interested in physics."

Jiang went on to study physics at Nanjing University in China, where he received his bachelor's degree before earning a master's and a doctorate in physics from Indiana University at Bloomington. He came to ORNL as a postdoctoral researcher and now is a staff scientist in the Neutron Technologies Division, where he's part of a group that develops neutron polarization techniques.

Using ORNL's High Flux Isotope Reactor and Spallation Neutron Source, Jiang is developing a device that can fully control neutron beam polarization — based on the spin of neutrons — and analyze complex magnetic structures. The development of an advanced spherical neutron polarimetry method could reveal new knowledge in complex magnetic materials that traditional methods have been unable to provide. Advancing research into quantum materials, for instance, requires a deeper understanding of magnetism.

"Spherical neutron polarimetry enables us to map the full picture of the neutron polarization vector during the scattering process," Jiang said. "This work will enhance our neutron facilities because we're developing the most advanced techniques in the world."

Jiang first began working in neutron scattering with his advisor at Indiana University's Low Energy Neutron Source. He said that working with world-class instruments at HFIR and SNS drives him to continue to expand his knowledge.

"Physics is a fascinating world to me. There is so much that is unknown. You never know when the theoretical world and the experimental world will connect," he said. "New discoveries can be anywhere."

The first step in his project is to deploy the polarimetry technique within several instruments at HFIR. Next, the capability will be expanded to SNS, which will be a unique challenge, as spherical neutron polarimetry has never been applied on a time-of-flight instrument — that is, one that collects measurements based on how long an object, particle or wave takes to travel a distance through a medium.

"The instruments are always evolving, and the need for better technique is always there. This keeps me going," Jiang said. "I want to see what using this new technique can do, what kind of things I can achieve, what kind of new science I can do."

An unanswered question launches a career quest

Elijah Martin

by Karen Dunlap
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Elijah Martin vividly remembers the first time he heard the word "plasma."

His 11th grade chemistry teacher at Hendersonville High School in Hendersonville, North Carolina, Frederick Van Itallie — Dr. V.I. to his students — was explaining the states of matter to the class.

"He was going through the phases of matter — 'A solid will impart more energy into a system, and it will turn into a liquid; add a little bit more energy to get a gas; add a little bit more beyond that, it will transition to a plasma,'" Martin recalls. "And I raise my hand and ask, 'What's plasma?'"

Perhaps Dr. V.I. didn't hear him ask, but Martin didn't get an answer, and it launched him on a journey that continues today. Plasma, he discovered, is a highly ionized gas containing an approximately equal number of positive ions and negative electrons.

"For the first time in my life, I went to the library on my own accord and looked it up," he said. "It was like a switch flipped in my head, and I knew I was going to spend the rest of my life studying this."

Martin credits his Christian faith for keeping him focused on his scientific pursuit.

"I feel very lucky that I found my path and I own that up to God," he said.

He went on to study physics and nuclear engineering at North Carolina State University, earning two bachelor's degrees. He completed his doctorate in nuclear engineering in 2014, also from NC State.

Now a scientist in ORNL's Fusion Energy Division, Martin seeks to investigate and quantify radiofrequency wave absorption phenomena that occur in edge plasma through a combination of novel laser-based spectroscopy and advanced quantum mechanical modeling.

For the past several years, Martin has been developing and assembling a first-of-its-kind laser-based diagnostic tool that can study the underlying physics at work. The next step is to scale that diagnostic tool to operate in the DIII-D National Fusion Facility in San Diego so measurements can begin in spring 2021, coinciding with the installation of a new radiofrequency antenna.

"Because of this tool, we'll be able to study physics at a level that is 10 times more advanced than anyone has done before," he said.

The diagnostic system will beam a precisely tuned laser across a band within the plasma and will map the electronic quantum mechanical information of the atoms present. Using data he collects to refine predictive computational models, Martin aims to provide insights that could accelerate progress toward continuous operation of fusion reactors.

"It's exciting to think that we could take the process that's going on in the sun and control it to generate power," he said.

Shifting from physics to ecology

Benjamin Sulman

by Karen Dunlap
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Estuarine wetlands — ecosystems where land meets rivers and oceans — host a complex, ever-shifting array of biogeochemical processes that affect the storage and processing of nitrogen and carbon in the soil and their release to the environment.

Benjamin Sulman, a scientist in ORNL's Environmental Sciences Division, seeks to fully assess this multidimensional system by simulating the environment using the Energy Exascale Earth System Model, a DOE leading-edge modeling, simulation and prediction project involving eight national labs, including ORNL.

Sulman credits exposure to a wide range of scientific fields and a cadre of mentors during his academic career for preparing him to tackle the complexity of modeling wetland ecosystems.

"The fact that I'm able to work in this area of ecology is due to learning from a lot of really talented people," he said. "I've built a basic skill set in developing environmental models, and now I can pivot those tools to work with different people and on different kinds of problems. Learning something new all the time makes research really exciting and enjoyable."

During his undergraduate program in physics and astronomy at Oberlin College in Ohio, Sulman began learning data analysis and computer coding. Shifting toward applied physics during his graduate work at the University of Wisconsin, Madison, he began exploring atmospheric and oceanic sciences, specifically interactions between ecosystems in the atmosphere, such as carbon dioxide exchange and how ecosystems affect turbulence and movement of air. His doctoral work, completed in 2012 at UW Madison, examined how wetland ecosystems exchange carbon dioxide with the atmosphere and how atmospheric changes affect wetlands.

Next, Sulman held postdoc appointments at Princeton University and Indiana University, where his work focused on environmental carbon cycle modeling with a focus on soils. He joined ORNL two years ago, where he has conducted ecosystem modeling of Arctic tundra plants and soil carbon processes.

"Arctic tundra processes and coastal wetland processes have some things in common: They're not well represented in models, and they both have many complex chemical processes at play," Sulman said. "Wetlands are dynamic; they are the intersection of all these different processes — dry soil, underwater soil, the chemical makeup of fresh water and salt water, vegetation. They're all interacting with each other."

Sulman's aim by the end of his five-year early-career project is to merge coastal data from the continental United States into one model that tracks how water flows from inland to the coasts as it goes through wetlands and how that influences the ocean near the United States. Having a comprehensive model can help make sense of how sudden changes, like hurricanes and wildfires, affect the nation's wetlands and oceans.

"It's increasingly important to understand how these ecosystems work," Sulman said. "Catastrophic events in an ecosystem are missing from a lot of current models."

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.

Joel Brogan

Postdoc, Electrification and Energy Infrastructures Division
Ph.D., Computer Science and Engineering, University of Notre Dame
Hometown: Orange City, Iowa

What are you working on at ORNL?

I'm working on developing virtual reality environments for data visualization and machine learning explainability. The goal is to have tools to understand why machine learning algorithms make the choices they do when analyzing complex signals in images and videos.

What would you like to do in your career?

I would like to be a part of the effort to solve complex machine learning problems that have the potential to revolutionize industry, commerce and security for the greater good. At the end of the day, I want to see that the work I am doing is helping people.

Why did you choose a career in science?

Science was not popular in my small town. In high school, I took a calculus class almost as a fluke and learned that I was good at it. My teacher was fantastic and made me feel supported; that was my gateway into engineering. Then, in college, I discovered a knack for computer programming.

Madalynn Marshall

Graduate student, Neutron Scattering Division
Ph.D. student, Chemistry, Rutgers University
Hometown: Mount Vernon, Iowa

What are you working on at ORNL?

I use neutron diffraction to study the magnetic structure of new quantum materials that can host both magnetism and exotic electronic properties. The resulting magnetic structures may reveal insight into any connection between the electronic and magnetic behavior in these materials.

What would you like to do in your career?

I would like to continue working with diffraction techniques in research to explore new materials and understand how they function at the atomic level.

Why did you choose a career in science?

I chose a career in chemistry largely due to the professors and peers I had as an undergraduate at Iowa State University. I was inspired by the concepts and driven by the challenges. I knew I was in the right field when chemistry started to feel like an old friend.

Yadukrishnan (Yadu) Sasikumar

Postmaster's researcher, Nuclear Energy and Fuel Cycle Division
Ph.D. student, Nuclear Engineering, The Open University, UK
Hometown: Thrissur, India

What are you working on at ORNL?

My research focuses on how used nuclear fuel interacts with water in the event of an accident in which the fuel gets exposed to the environment. I use experimental techniques such as mass spectrometry and microscopy to understand changes in behavior of spent fuel samples exposed to water and steam.

What would you like to do in your career?

I believe that nuclear has a major role to play in our energy mix and would like to continue my research in strengthening the long-term management of used fuels. I have thoroughly enjoyed working at ORNL and aspire to have a career in a national laboratory environment such as here.

Why did you choose a career in science?

My parents were dedicated to science, and it didn't take me long to develop an interest in it. Growing up, I loved machines, which led me to an undergraduate degree in engineering. I subsequently took up nuclear, as I'm fascinated by its potential in solving the impending global energy crisis.

Erica Grant

Graduate student, Computational Sciences and Engineering Division
Ph.D. student, Quantum Computing, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Richmond, Virginia

What are you working on at ORNL?

I am solving real-world problems (like finding the optimal investment portfolio) with a quantum annealing machine that has the potential to solve computationally difficult problems with less energy or time. I use these problems to study the different tuning strategies and hardware controls that could improve the performance of the quantum annealer.

What would you like to do in your career?

I have started a quantum information technology and security startup: Quantum Lock Technologies. Outside my studies and research, I am building security solutions for access-control facilities by using completely random and unpredictable digital keys. I hope to improve security on a global scale by utilizing quantum technology.

Why did you choose a career in science?

I enjoy gaining a deeper understanding of our universe and working with cutting-edge technology to develop new and innovative solutions.

Miguel Toro Gonzalez

Postdoc, Radioisotope Science and Technology Division
Ph.D., Mechanical and Nuclear Engineering, Virginia Commonwealth University
Hometown: Medellín, Colombia

What are you working on at ORNL?

I study how nanoparticles can be designed and used to deliver alpha-emitting radionuclides for treatment of cancer and infectious diseases. My research involves assessing the radionuclide encapsulation, tailoring the surface chemistry for specific targeting, and understanding the radiobiology of radioactive nanoparticles.

What would you like to do in your career?

I would like to work in research to advance the field of targeted radionuclide therapy for cancer treatment by using nanomaterials as delivery platforms. I would like to develop expertise in designing radiopharmaceuticals and understanding their radiobiology to enhance the treatment of cancer and infectious diseases.

Why did you choose a career in science?

Science is an endless loop of experiments, failures, successes and discoveries that can revolutionize the way we live and see life. Science has allowed me to study, explore and combine different fields to solve problems and develop new applications and technologies that can have a positive impact in the world.

Sara Isbill

Postdoc, Nuclear Nonproliferation Division
Ph.D., Chemistry, University of Tennessee
Hometown: Madisonville, Tennessee

What are you working on at ORNL?

My research primarily involves computational modeling of defective carbon fiber structural units to relate experimental measurements to the atomic-level structure for improved understanding of how defects alter carbon fiber properties.

What would you like to do in your career?

I want to advance our understanding of the world around us, though I'm not yet sure where my scientific journey will take me over the course of my career. I currently plan to continue doing research but have not ruled out career options such as teaching or program management.

Why did you choose a career in science?

I found my high school and college chemistry classes to be the most challenging but enjoyable courses I took, motivating me to continue learning more about this field. A career in science allows me to continue learning about new systems and techniques and apply that knowledge to exciting research problems.

The barn that wasn't a barn

by Leo Williams
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In 1948, the government erected a funny-looking building in the woods between ORNL and the Y-12 Plant (now the Y-12 National Security Complex). Named Installation Dog, it was a concrete bunker built into the side of a hill, with a vault that would do a bank proud.

What made it look odd was the view from the outside. Installation Dog was masked with the walls and roof of a barn, and a nearby silo was in fact a machine gun nest. But while its rustic facade and tight security might have looked a little bizarre to someone on the ground, from the air it was indistinguishable from the many barns that dotted the region, and that was the point.

Installation Dog stored highly enriched uranium. This was a time when the United States was the only country in the world to have nuclear weapons, and the government needed secure, secret storage.

And it was indeed secret. Even the draftsman who designed the structure was not told what it was for. The site was patrolled day and night, and its alarm system was so sensitive that it was periodically triggered by wild animals.

Installation Dog served its intended purpose for only a year, from May 1948 to May 1949. It was kept under guard for several more years—just in case—but its days storing uranium were over.

Fortunately, the following decade brought the site a new purpose—and a new name. The purpose came from the Analytical Chemistry Division, which took over Installation Dog in the late 1950s and early '60s and put it to work as a laboratory. The building's new name came from the division director's secretary, Katherine Odom, who was fond of taking her lunch there. In her honor, Installation Dog became Katy's Kitchen, a name that has stuck, albeit informally, ever since.

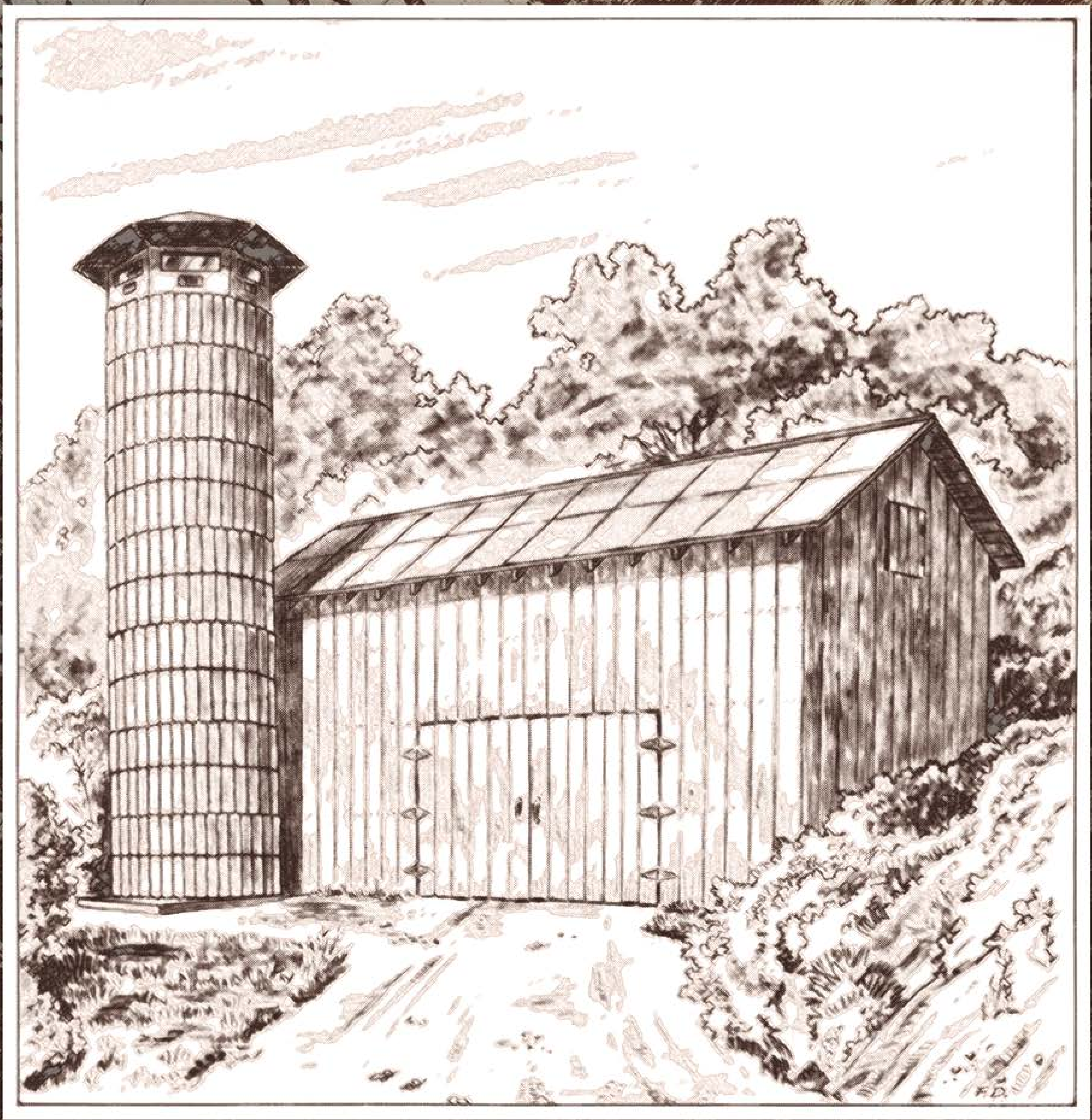
Katy's Kitchen spent its most prolific years with the Environmental Sciences Division, which occupied it from the 1970s through 2013. In the early years, the concrete bunker served as a field chemistry laboratory and storage space. In later years, a new building was constructed in front of the bunker, and the original vault door was removed for safety reasons.

The building known first as Installation Dog and later as Katy's Kitchen has served a variety of purposes over the last seven decades. Image credit: ORNL

One of the scientists using Katy's Kitchen was Paul J. Hanson, now a Corporate Fellow in the Environmental Sciences Division. In a brief compiled history of the site, he notes that it supported a variety of environmental projects, including:

- Studies in the 1970s and 1980s of biogeochemistry in the Walker Branch Watershed, a small watershed east of ORNL's main campus adjacent to Katy's Kitchen.
- DOE's Atmospheric Radiation Monitoring Program, which in the mid-1990s used the newer building to analyze meteorological phenomena and solar radiation to get a better handle on climate change.
- The Throughfall Displacement Experiment, which ran for 15 years in the 1990s and 2000s and studied the implications of changing rainfall to the ecosystem.
- The Enriched Background Isotope Study project, which ran from the late '90s through 2013. The study took advantage of a local rise of background radioactive carbon-14 — the isotope used for carbon dating — to study the journey of carbon through plants and soil.

Katy's Kitchen has gone unused since the mid-2010s as ORNL's environmental research focus moved off the Oak Ridge Reservation. But memory of the site that went from secret storage space to makeshift lunchroom to environmental laboratory lives on.



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