OAK RIDGE NATIONAL LABORATORY

Review

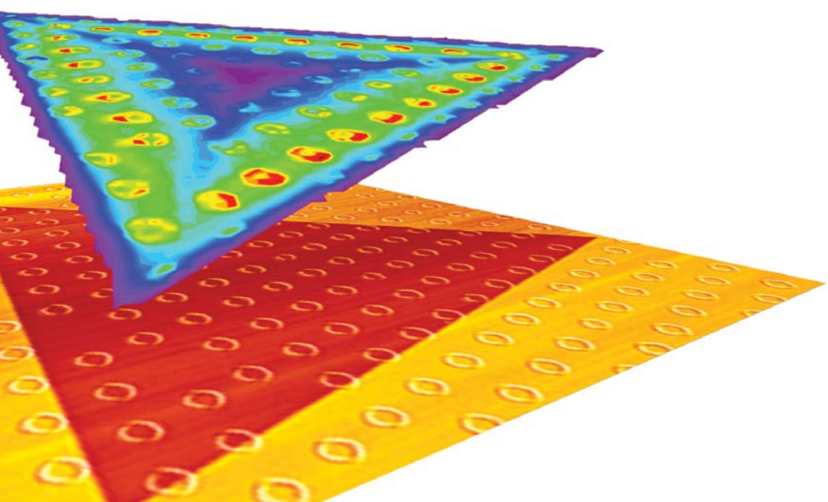
Harvesting carbon:

OAK RIDGE National Laboratory

Vol. 53 | No. 3 | 2020
www.ornl.gov/ornlreview

OAK RIDGE NATIONAL LABORATORY
Review
Vol. 53 | No. 3 | 2020

Contents



On the Cover

ORNL nanoscientist Rigoberto Advincula.
Image credit: Carlos Jones, ORNL

Applying diverse expertise at a global scale

At Oak Ridge National Laboratory, we translate fundamental research into applications with worldwide impact. This issue of *ORNL Review* highlights discoveries and projects across our broad portfolio that illustrate our multidisciplinary approach to some of the world's most difficult scientific and technical challenges.

Among our grandest challenges is the ability to harness fusion energy to produce electricity. Scientists and engineers have long sought to produce net energy for the grid by sustaining reactions among abundant hydrogen isotopes in a burning plasma. When they succeed, it will truly transform the world by enabling safe, virtually limitless energy.

ORNL manages U.S. contributions to the world's largest fusion experiment—the ITER project, under construction by seven international partners in France—but taking ITER's technology to a commercial scale requires materials able to withstand conditions hotter than the core of the sun. We are tackling this problem with our Material Plasma Exposure eXperiment — or MPEX —a linear plasma device for studying the long-term interactions between fusion devices and the materials that must withstand these extreme environments (see "New device will test materials for fusion reactors," page 26).

In another arena of ORNL research—materials, computing, and information transfer—the mastery of quantum behavior promises transformative breakthroughs, too. Just as the invention of the transistor and microprocessors brought the world into the Information Age, the next sea change will come from quantum technology, and ORNL is at the forefront.

Our strategy for growing atomically thin 2D crystals that cling to 3D objects points the way to better single photon emitters for next-generation electronics (see "Curved crystals are promising for quantum devices," page 32). Researchers from ORNL and Los Alamos National Laboratory also used quantum key distribution to substantially increase the range covered by quantum technologies (see "Quantum technologies go the distance," page 24), which holds promise for the cybersecurity, longevity and efficiency of the nation's power grid. And in August, DOE awarded ORNL $115 million over five years to lead the Quantum Science Center with partners including Caltech, Harvard, and IBM (see "ORNL picked to lead new Quantum Science Center," page 2).

Fusion and quantum represent new frontiers—entirely new approaches that will ultimately impact everyone in the world—but our researchers are hard at work on a more immediate world-wide concern, too: the COVID-19 pandemic.

This issue explains how ORNL staff members and researchers from other institutions are using the lab's Summit system — the most powerful US supercomputer — to study the SARS-CoV-2 virus (see "Record-breaking supercomputer simulations aid COVID-19 research," page 20). There are more than 20 computing projects in all.

One team used Summit to screen 1.5 billion chemical compounds over the course of 24 hours, the largest drug-screening study ever done on a supercomputer. Another project compared lung fluid cells from COVID-19 patients with a control group, looking at gene expression and co-expression patterns, while still another looked at gene expression patterns for 700,000 combinations of existing drugs.

Finally, this issue of *ORNL Review* looks at efforts to help bring the Earth's carbon cycle into balance—a grand scientific challenge requiring leadership in areas as varied as the physical sciences, artificial intelligence and data analysis, neutron research and biological and environmental sciences (see "Balancing carbon: ORNL sets its sights on a global challenge," page 6).

I hope you enjoy updates on these initiatives and others across the laboratory in this issue of *ORNL Review*.

Thomas Zacharia
Laboratory Director

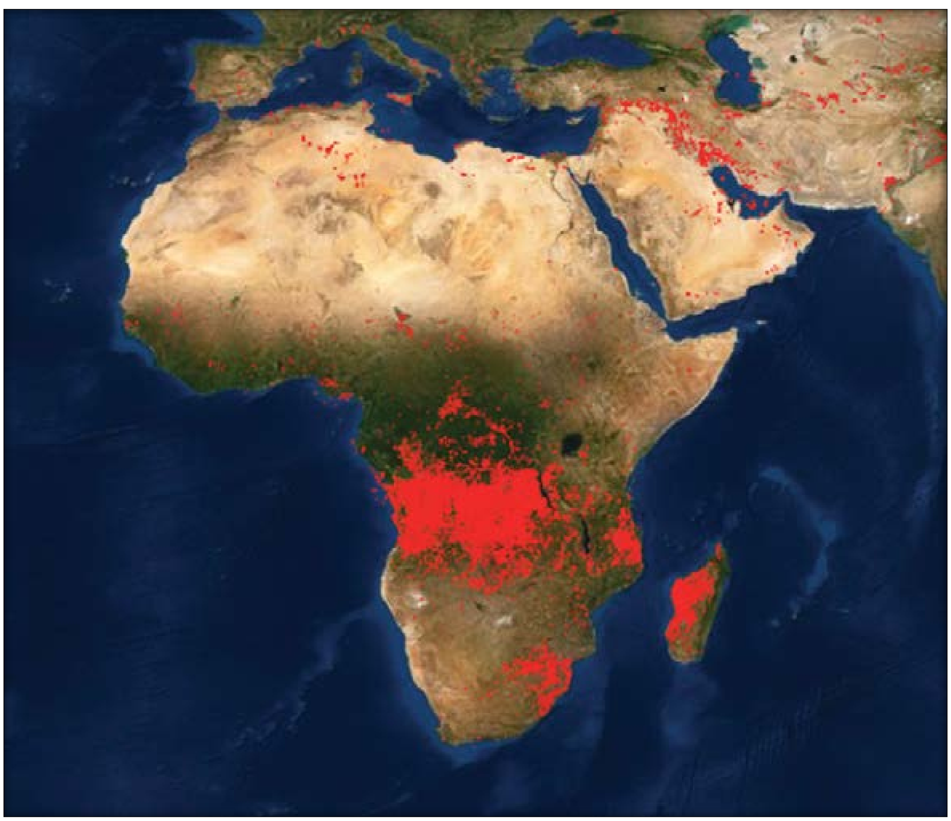
Machine learning predicts fire risk in Africa

ORNL researchers developed a method that uses machine learning to predict seasonal fire risk in Africa, where half of the world's wildfire-related carbon emissions originate.

Their approach draws on data about underlying environmental drivers such as ocean temperatures and land surface changes in addition to more commonly used atmospheric and socioeconomic indicators. The method allows scientists to gain a deeper understanding of the relative importance of different variables such as soil moisture and leaf area.

"We found that oceanic and terrestrial dynamics are the most critical factors influencing the accuracy of seasonal fire prediction for these vulnerable ecosystems," said ORNL's Jiafu Mao. "Disturbances like fire can have a lasting impact on regional environments and global carbon cycling."

The scientists' computational framework could be applied to other regions or generalized to assess global fire risk and inform fire management practices that address environmental and safety concerns.—*Kim Askey*



ORNL developed a method that uses machine learning to predict seasonal fire risk in Africa, where half of the world's wildfire-related carbon emissions originate. Image credit: NASA

ORNL picked to lead new Quantum Science Center

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

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

The Quantum Science Center, led by ORNL, will receive $115 million over five years from DOE's Office of Science to realize the potential of topological quantum materials for manipulating, transferring and storing quantum information. Quantum materials exhibit exotic properties under specific conditions, and the center will transition this knowledge to the private sector for use in practical applications such as quantum computers and sensors.

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. The center's 16 partners include Harvard University, Caltech and IBM.

"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."—*Scott Jones*

ORNL tech advances used to charge UPS truck

ORNL researchers have demonstrated a 20-kilowatt bi-directional wireless charging system installed on a UPS medium-duty, plug-in hybrid electric delivery truck.

The project is the first of its kind to achieve power transfer at this rate across an 11-inch air gap, advancing the technology to a new class of larger vehicles with higher ground clearance.

ORNL's wireless charging technology transferred power between the truck and a charging pad across the 11-inch gap using two electromagnetic coupling coils at the demonstration. The system transferred electricity from the power grid to the vehicle battery terminals at more than 92 percent efficiency.

At a 20-kilowatt level, it would take about three hours to charge the vehicle's 60-kilowatt-hour battery packs. Conventional wired charging typically takes five to six hours using the existing onboard charging system.

With its bi-directional design, the system also supports use of the vehicle's batteries for energy storage. Doing so would give energy flexibility to a fleet owner's business and help better manage on-site generation such as solar power. ORNL's bidirectional technology is fully compliant with grid power quality standards.

"Scaling the technology to a fleet of 50 trucks gives you megawatt-scale energy storage," noted ORNL's Omer Onar, who led the technical team's effort at the lab.

The technology takes energy from the grid and converts it to direct current voltage. Then a high-frequency inverter generates alternating current, which in turn creates a magnetic field that transfers power across the air gap. Once the energy is transferred to the secondary coil across the air gap, it is converted back to DC, charging the vehicle's battery pack.

The system incorporates ORNL's custom electromagnetic coil design and controls system, as well as wide bandgap power conversion systems. The technology was tested using grid and battery emulators before integration into the vehicle, utilizing two unique facilities at ORNL: the DOE National Transportation Research Center user facility and the lab's Grid Research Integration and Deployment Center.—*Stephanie Seay*

ORNL's Bianca Haberl and Amy Elliott hold 3D-printed collimators—an invention that has been licensed to ExOne, a leading binder jet 3D printer company. Image credit: Genevieve Martin, ORNL

ORNL licenses 3D-printed neutron scattering tech

ORNL has licensed a novel method to 3D print components used in neutron instruments for scientific research to the ExOne Company, a leading maker of binder jet 3D-printing technology.

A long-time collaborator with ORNL, ExOne will leverage the lab's world-class expertise in additive manufacturing, materials and neutron science to further develop the patent-pending technique to 3D print collimators using a lightweight, metal-infused composite that is ideal for neutron scattering instruments.

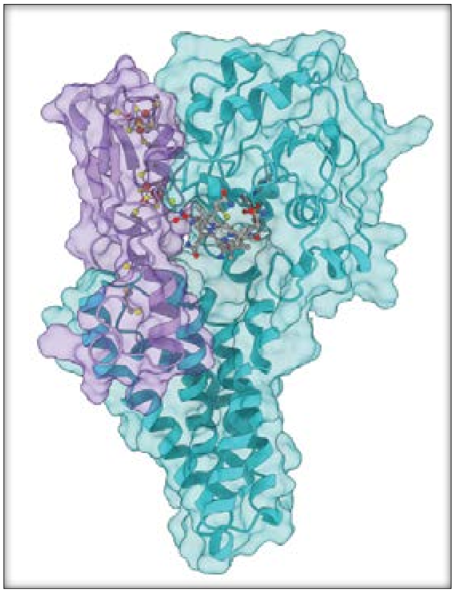
ExOne intends to scale up production of neutron-friendly collimators—the company's first opportunity to offer high-quality, lower-cost components for neutron beamline applications.

Similar to an aperture in a camera, collimators help to precisely define the neutron beam, a function that provides higher-fidelity measurements of a sample's atomic and molecular structure and dynamics.

"Our work on collimators has been focused on tungsten infiltrated with copper for use in X-ray machines, computed tomography, or CT, scans and magnetic resonance imaging machines, or MRIs," said Dan Brunermer, ExOne technical fellow. "The technology we have licensed from ORNL will allow us to build collimators for neutron scattering, and that requires a specialized mix of materials and postprocessing."—*Sara Shoemaker*

For more information: go.usa.gov/xfKrS

ORNL researchers demonstrated a 20-kilowatt, bidirectional wireless charging system on a medium-class hybrid electric delivery truck. Image credit: Brittany Cramer, ORNL



A structural model of HgcA, shown in blue, and HgcB, shown in purple, was created using metagenomic techniques to better understand the transformation of mercury into its toxic form, methylmercury. Image credit: Connor Cooper, ORNL

Protein models explore methylmercury formation

An ORNL-led team has created a computational model of the proteins responsible for the transformation of mercury to toxic methylmercury, marking a step forward in understanding how the reaction occurs and how mercury cycles through the environment.

Methylmercury is a potent neurotoxin that is produced in natural environments when inorganic mercury is converted by microorganisms into the more toxic, organic form. In 2013, ORNL scientists announced a landmark discovery, identifying a pair of genes, hgcA and hgcB, that are responsible for mercury methylation.

Those genes encode the proteins HgcA and HgcB, whose structure and function ORNL scientists have been working to better understand.

"We don't have an experimental structure yet for these proteins, so the next best thing is to use computational techniques to predict their structure," said head investigator Jerry Parks.

The computational model was generated using a large dataset of HgcA and HgcB protein sequences from many different microorganisms, ORNL's high-performance computing resources and bioinformatics, and structural modeling techniques as detailed in a recent article in *Communications Biology*.

The result is a 3D structural model of the HgcAB protein complex and its cofactors that scientists can use to develop new hypotheses designed to understand the biochemical mechanism of mercury methylation and then test them experimentally.—*Stephanie Seay*

ORNL's Juergen Rapp named ANS fellow

Juergen Rapp, a distinguished R&D staff scientist in ORNL's Fusion Energy Division, has been named a fellow of the American Nuclear Society in recognition of his contributions to the advancement of nuclear science and technology.

ANS stated that the society recognizes Rapp "for technical leadership in fusion plasma surface interactions, including the development of impurity seeding to mitigate fusion power exhaust, and in the development of experimental facilities for studying plasma surface interactions at Magnum-PSI (Netherlands) and proto-MPEX (USA)."

Juergen Rapp

Rapp is a scientific leader of the Material Plasma Exposure eXperiment, a linear plasma device used for the analysis of advanced materials necessary for experimental fusion reactors such as the multinational ITER experiment. In recognition of his leadership of the facility and for his work in power exhaust and plasma material interactions in fusion, he was named a fellow of the American Physical Society in 2017.

Rapp joined the Lab in 2011 where he began developing the MPEX project. Prior to ORNL, he worked at the FOM Institute for Plasma Physics in Nieuwegein, The Netherlands; the Joint European Torus at Culham, UK; and the Research Center in Juelich, Germany.—*Karen Dunlap*

ORNL's Ozpineci wins society achievement award

Burak Ozpineci of ORNL's Buildings and Transportation Science Division has won the 2020 IEEE Power Electronics Society Vehicle and Transportation Systems Achievement Award.

Ozpineci was cited for his contributions to the "advancement of power electronics in transportation electrification and wireless charging of electric vehicles." The award recognizes innovators and researchers who have made outstanding technical contributions to the use of power electronics in vehicle and transportation systems.

Ozpineci leads the Vehicle and Mobility Systems Section and manages the Electric Drive Technologies Program at ORNL. He is also an IEEE Fellow.

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

Burak Ozpineci

ORNL's Peter honored by manufacturing society

The Society of Manufacturing Engineers has named William Peter of ORNL's Manufacturing Demonstration Facility among its 2020 College of SME Fellows.

SME is a professional association dedicated to advancing manufacturing technology and education. This honor recognizes Peter's significant contributions to manufacturing and is reserved for those with more than 20 years of noteworthy work in the field.

Peter said he hopes to bring attention to "the most pressing, fundamental challenges that the U.S. manufacturing sector is facing."

"By being a fellow, I can help to shine a light on the wonderful research being performed at ORNL and our work with industry and academia in additive manufacturing, composites, machining, roll-to-roll processing, digital fabrication and automation," he said.

A leading voice for advancement and opportunity in manufacturing, SME offers resources for manufacturers, promotes advanced manufacturing technology and works to develop a skilled workforce. Peter and the MDF team have a long-standing relationship with the organization and contribute to its educational events and conferences.

"SME is a vital platform for us to communicate breakthroughs in advanced manufacturing through their large membership," Peter said.—*Karen Dunlap*

ORNL Manufacturing Demonstration Facility's Bill Peter has been named to the 2020 College of SME Fellows. Image credit: Carlos Jones, ORNL

ORNL's Perumalla to lead ACM simulation groups

ORNL's Kalyan Perumalla has been elected chair of the Association of Computing Machinery's Special Interest Group on Simulation.

Kalyan Perumalla

According to the organization's website, ACM is the "world's largest educational and scientific computing society" and "brings together computing educators, researchers, and professionals to inspire dialogue, share resources, and address the field's challenges."

ACM's 37 Special Interest Groups aim to advance innovation in computing's major subfields via networking, continued education, and numerous other functions.

Specifically, SIGSIM co-sponsors major international conferences such as the Winter Simulation Conference and the Conference on Principles of Advanced Discrete Simulation, recognizes leading research via Distinguished Innovation Awards, provides support for students to travel to major events and hosts a social network on LinkedIn, among other activities supporting the worldwide simulation community.

Perumalla cited two primary motivations for his desire to lead the group: giving back to the community and setting the stage for the next decade.

He's been involved with SIGSIM for over 20 years; in fact, the first paper he submitted to the organization's flagship international workshop in 1999 won the Best Paper Award. "I couldn't pass up the opportunity to lead this professional community I've been a part of for so many years," he said.—*Scott Jones*

Balancing carbon:

ORNL sets its sights on a global challenge

by Leo Williams
williamsjl2@ornl.gov

Carbon is an exceptionally useful element, to say the least. That pound of sugar in your cupboard contains nearly seven ounces of carbon. Assuming you weigh 150 pounds, your own body contains 27 pounds of carbon. And the diamond on your wedding ring is made entirely of carbon.

Steel needs carbon, as do plastics and other polymers. Even your own DNA wouldn't exist without carbon.

But too much of this indispensable element in the wrong place can be a problem. That's what we face with the Earth's carbon cycle—a term that refers to the exchange of carbon among the planet's oceans, atmosphere, plants and soil.

Our atmosphere in particular has more carbon—in the form of carbon dioxide—than at any time in the last 3 million years, primarily due to the burning of coal, gasoline and other fossil fuels. In fact, the level of CO_2 in our atmosphere has risen by a quarter in just the last 45 years.

Facing the problem head-on

This imbalance is the focus of an ORNL effort entitled "Balancing the Carbon Cycle"—a focus area that in the coming years will develop technologies to pull excess CO_2 out of the atmosphere and other sources, as well as carbon contained in biomass and polymers, and turn it into valuable materials, thereby truly conserving carbon as a resource to enable production of valuable new materials.

"There is an incredible imbalance in the carbon cycle right now," noted ORNL Corporate Fellow Bobby Sumpter, who is leading the effort. "It will require a lot of effort and a lot of creativity."

The ORNL carbon focus is a recognition not only of the problems associated with carbon in the atmosphere, but also of the cost of squandering this valuable resource, noted Michelle Buchanan, the lab's deputy for science and technology.

"I was at a meeting back a few years ago," she said, "and a guy from a major oil company got up and said if all we do is burn carbon, we're in trouble, because if we run out of easy-to-get, cheap carbon, you're not going to have polyester carpets, you're not going to have baby diapers, you're not going to have Saran

> “There is an incredible imbalance in the carbon cycle right now. It will require a lot of effort and a lot of creativity.
> — ORNL Corporate Fellow **Bobby Sumpter**

Wrap, you're not going to have tables that have a plastic coating on the top. And so we need to think about saving those carbons and reusing them.”

ORNL is in a unique position to address the problem. With world-class experimental centers, the country's fastest supercomputer and expertise across the gamut of physical sciences and engineering, artificial intelligence and data analysis, the lab has the tools necessary to take a comprehensive look at the Earth's carbon cycle and devise strategies to bring it back into balance.

To be effective, Sumpter said, the project will require coordination among chemists, chemical engineers, physicists and biologists, as well as experts in artificial intelligence, machine learning and data analysis.

New strategies

The effort—a “science of the future” approach— will incorporate at least two new research strategies. First, individual projects will be tightly coordinated, from nanoscale explorations of new catalysts to scale-up of potential solutions.

“The difference between the science of the future approach and typical approaches,” Sumpter said, “is that we will take advantage of expertise that crosscuts everything from chemistry, physics, materials science and engineering, to computer science and applied mathematics, all the way through to ‘at-scale engineering’.”

With the carbon focus area, for example, efforts to create new catalytic materials and membranes will be undertaken with a

See BALANCING CARBON: ORNL SETS ITS SIGHTS, page 8

Bobby Sumpter. Image credit: Carlos Jones

BALANCING CARBON: ORNL SETS ITS SIGHTS, page 7

close eye on how these materials would fit into a deployment of hundreds or even thousands of industrial facilities.

"We have the talent," Sumpter said, "but we often tend to work on specific pieces of our own disciplines in isolation and don't truly integrate the pieces together that are required to solve such a grand challenge problem. The old adage is highly pertinent: The whole needs to be greater than the sum of the parts."

ORNL physical chemist Shannon Mahurin. Image credit: Carlos Jones

"Right now, basically you take a measurement, and you go back to your office for a week and interpret it," Buchanan said. "Then you go back and take another experiment, and you go back and interpret it."

"This could be an iterative thing where you would get all this information together, and the computer would help you with that decision."

Twofold approach

The carbon focus area will be divided into two coordinated thrusts.

Capture–separation–conversion. The first thrust area will develop technologies to capture carbon from the air, separate it from other gases and convert it into useful products or their precursors, all in one process (see "All-in-one carbon conversion," page 12).

Led by ORNL physical chemist Shannon Mahurin, this will be largely a materials science and chemistry effort. Catalysts, membranes and other materials will have to be developed that are far more effective than anything currently in use and that can work collaboratively to enable simultaneous efficient capture, separation and conversion.

Under this thrust area, carbon dioxide will no longer be treated as a waste product to be disposed of in underground reservoirs. Instead, it will be used as a valuable feedstock for fuels, high-level polymers and other products.

Polymer chemistry. The second thrust area will focus on the chemistry necessary to turn CO_2 and other carbon sources such as biomass and discarded (waste) polymers, into high-level polymers and other high-performance materials. (see "Making the most of captured carbon," page 14).

Among the most promising potential products for the captured carbon are materials that perform well under extreme conditions or that can be used to manufacture aircraft and automobiles or as feedstocks for 3D-printing applications.

> *"I was at a meeting back a few years ago, and a guy from a major oil company got up and said if all we do is burn carbon, we're in trouble, because if we run out of easy-to-get, cheap carbon, you're not going to have polyester carpets, you're not going to have baby diapers, you're not going to have Saran Wrap, you're not going to have tables that have a plastic coating on the top. And so we need to think about saving those carbons and reusing them.*
>
> — ORNL Deputy for Science and Technology **Michelle Buchanan**

Second, the carbon focus area will be guided from day one by the lab's expertise in artificial intelligence, machine learning, data analysis and automation. Data from neutron scattering or electron microscopy experiments, for example, will be analyzed as the experiments are being conducted, and the computers may even tweak experiments as they are being conducted. And at least one lab will be robotically controlled.

"If we know to look for a correlation, then we often have a statistical process to find it. But if we don't even know what to look for, how do we start? That's where machine learning excels.

— ORNL Director of Artificial Intelligence Programs **David Womble**

Milking data for all it's worth

Artificial intelligence and machine learning are this ORNL effort's not-so-secret weapons. Each thrust area will be supercharged by the lab's computational expertise and by facilities such as the Summit supercomputer and the lab's Compute and Data Environment for Science, or CADES.

According to David Womble, ORNL's director of artificial intelligence programs, machine learning will boost this effort in critical ways.

One is the ability to sift through enormous data sets and identify potential cause-and-effect relationships that can lead, for example, to better materials or processes. While human researchers are reasonably good at verifying relationships that they know to look for, it takes the data-handling power of modern supercomputers and advanced data mining techniques to find that unlooked-for needle in a haystack.

"Inside these data sets there are complex correlations that humans are not able to extract—or even know to look for," Womble said. "If we know to look for a correlation, then we often have a statistical process to find it. But if we don't even know what to look for, how do we start? That's where machine learning excels."

Simplifying the problem

Another strength of artificial intelligence is the ability to create surrogates for especially data-intensive portions of computational models, ones where brute-force computations based on the laws of physics are not feasible.

"First-principles models are sometimes so complex that they are computationally intractable, even on modern supercom-

See BALANCING CARBON: ORNL SETS ITS SIGHTS, page 10

BALANCING CARBON: ORNL SETS ITS SIGHTS, page 9

puters," Womble said. "AI is able to take data—both experimental and from simulation—and create a faster-running model."

The technique is especially valuable when a computation needs to address a wide range of scales. For example, Womble pointed to the creation of a unified system for capturing, separating and converting CO_2.

Ben Mintz, who leads ORNL Federated Instruments. Image credit: Carlos Jones

For such a system, researchers will need models that range from the scale of molecules in a membrane or catalyst to the scale of air or liquid flowing through that membrane or catalyst. These scales will vary by at least six orders of magnitude in both space and time, from microns to meters and microseconds to seconds.

First-principles models that look at each molecule individually cannot handle that range of scales, Womble noted, and continuum models that average the important values are not accurate enough. But machine learning models developed using both experimental and simulated data—while they may not give detailed information at the microscale—can provide accurate and computationally feasible approximations at the macroscale.

Getting machines to communicate

The other technical challenge will be the development of seamless communication among the computers and experimental facilities, an effort known as Connected Smart-Instruments.

At least one chemistry lab involved with the project will take this approach to its logical conclusion. The Autonomous Robot-Controlled Chemistry Laboratory—or ARC Lab—will replace humans with robotic controls able to speed the process of conducting and analyzing experiments.

The ARC Lab enables robots to become researchers with direct access to integrated theory, simulation and modeling, allowing the lab to analyze data and adjust experiments accordingly.

Ben Mintz, who leads ORNL Federated Instruments, said the ARC Lab will focus on catalysis research.

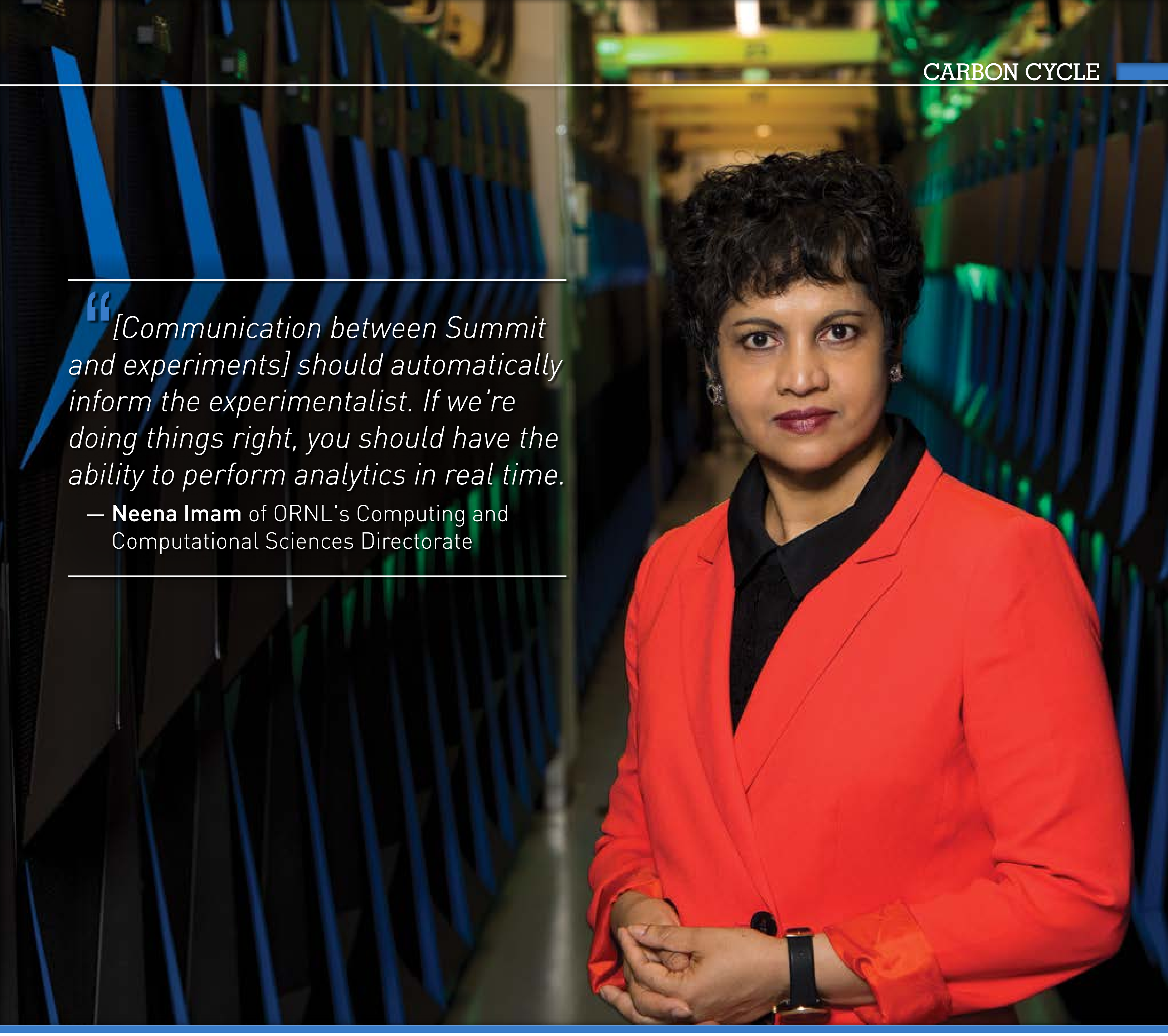
"We're going to build a lab that incorporates a robot capable of moving between stations to perform experiments," Mintz explained. "Anything that carbon cycle experimentalists need for catalysis—either liquid phase or solid phase—we're going to have the robot create them at a much faster rate."

Mintz noted that the lab will have its own computer—called an Edge Analysis Center. Plans call for a small-scale demonstration of the lab by the end of 2021, which will be followed by a more complex lab setup in the following years.

> *"The reason we think this is the right time and right place is that there's a lot of tools and expertise which previously were not available. Previously, it seemed unthinkable that machine learning could allow you to provide some realistic guidance in terms of what kind of material space you need to look into.*
>
> — Separations and Polymer Chemistry Section Head **Sheng Dai**

Experiments will also benefit from ORNL's high-performance computers, including Summit. With Summit talking to an advanced electron microscope, for instance, data can be analyzed as it's being collected.

"It should automatically inform the experimentalist," said Neena Imam, who leads research collaborations for ORNL's Computing and Computational Sciences Directorate. "If we're doing things right, you should have the ability to perform analytics in real time."



> *"[Communication between Summit and experiments] should automatically inform the experimentalist. If we're doing things right, you should have the ability to perform analytics in real time.*
>
> — **Neena Imam** of ORNL's Computing and Computational Sciences Directorate

Imam noted that the Connected Smart-Instruments initiative is not limited to ORNL. Instead, DOE is moving to connect resources throughout the agency's national laboratories and other facilities.

Womble agreed that coordination between computers and experimental equipment can accelerate research.

"As you are running your experiment and doing your analytics, you may see that you need to change some parameters. AI-based controls may be able to change a parameter without having to wait for an entire experiment to run and then do postexperimental data analytics."

The challenge, he said, is not to develop the needed expertise. That is already on hand. The challenge is simply to integrate the lab's world-class researchers and world-class equipment to work together concurrently toward a common goal.

The time for this coordination is now, experimentalists and computer experts strongly agree.

ORNL Separations and Polymer Chemistry Section Head Sheng Dai pointed to the powerful tools that will be employed by this effort, from supercomputing resources to world-class neutron scattering facilities to state-of-the art electron microscopes.

"The reason we think this is the right time and right place is that there's a lot of tools and expertise which previously were not available," Dai said. "Previously, it seemed unthinkable that machine learning could allow you to provide some realistic guidance in terms of what kind of material space you need to look into.

"All these new tools allow us to dig more deeply into the fundamental processes happening in these systems, which may lead us to some really high-impact discoveries."

All-in-one carbon conversion

by Leo Williams
williamsjl2@ornl.gov

Researchers have been working for years to develop technology that pulls carbon dioxide out of the air.

For the most part, this work has been in the form of one-off projects conducted by relatively small research teams, with little regard to how they might be scaled up or how the carbon might be repurposed.

ORNL's carbon effort and its combined carbon capture–separation–conversion focus area will take a different approach, coordinating physical experiments with one another and with the lab's formidable computing muscle.

> *"There are certainly foundations that we can build from. There's been a lot of work on the separations process. For example, we know a lot of different materials that will either selectively bind or transport CO_2, as a membrane or as an absorber.*
>
> — ORNL physical chemist **Shannon Mahurin**

Researchers will develop technology to—in the same process—remove carbon dioxide from the atmosphere, separate it from other gases and convert it into valuable products. Along the way, the project will incorporate insights from research being conducted to turn the carbon into high-level polymers (see "Making the most of captured carbon," page 14).

"Most other places working on this are taking a more mom-and-pop approach," said Sheng Dai, leader of the lab's Separations and Polymer Chemistry Section. "At Oak Ridge, we're approaching it as an interdisciplinary problem. We have materials scientists, we have chemists, we have engineers and chemical engineers, and everyone brings to the table a different expertise."

ORNL also has some of the world's most powerful scientific tools. These include experimental facilities such as the neutron scattering resources of the Spallation Neutron Source and High Flux Isotope Reactor and the electron microscopes and other advanced instruments at the Center for Nanophase Materials Sciences. They also include world-class computing tools such as the country's most powerful supercomputer, Summit, and the Compute and Data Environment for Science, or CADES.

The growing power of artificial intelligence and machine learning will be crucial to the project's success. It will guide new research, of course, analyzing data as it's being produced and creating and testing hypotheses. But it will also apply the power of artificial intelligence and data analysis to research that has been conducted in the past at ORNL and elsewhere, sifting through a mountain of data in search of new insights.

"There are certainly foundations that we can build from," explained ORNL physical chemist Shannon Mahurin, who will be leading the research effort. "There's been a lot of work on the separations process. For example, we know a lot of different materials that will either selectively bind or transport CO_2, as a membrane or as an absorber."

The project will also benefit from seamless communication between ORNL's computing systems and experimental tools such as neutron scattering instruments and advanced microscopes. This coordination will allow researchers to analyze experiments as they are being conducted and even tweak them as they are taking place.

Pushing the ball forward

The carbon project will need all of these advantages to push the technology much farther than anything seen so far. Research to date has focused primarily on removing CO_2 from flue gases at power plants or other carbon-intensive facilities. The potential for pulling CO_2 directly out of the air has been studied less extensively.

"If I can, I'll quote Kennedy, who said we go to the moon not because it's easy, but because it's difficult. That's the reason we really need a holistic approach toward this complex problem.

— ORNL Separations and Polymer Chemistry Section Head **Sheng Dai**

It's a much harder job. A power plant's flue gas can contain upwards of 10 percent CO_2; in contrast, CO_2 levels in the atmosphere are a little over 400 parts per million (or about 0.0004 percent). That level may be enough to bring the carbon cycle out of balance, but it's minuscule when you're talking about harvesting it from the atmosphere.

"From a chemistry perspective, this is tiny," Dai said. "It's like searching for a needle in a haystack. The sorbent needs to be very selective, very smart, and have very high capacities."

The project is largely a materials challenge. Carbon capture relies on technologies such as sorbents, which pick up and hold a material, membranes, which allow some things through but not others, and catalysts, which enable chemical reactions but are not altered by them.

The researchers must find materials that very effectively bind CO_2 without binding to other gases—especially nitrogen and oxygen, which together make up about 99 percent of the air around us. Those materials must at the same time be able to release the carbon so that it can be converted into high-level polymers and other products.

In addition, the team must find materials to do the converting. And, as Dai noted, the scale of the effort dictates that any new catalysts must rely on abundant elements rather than platinum and other noble metals.

While the challenge of capturing and processing the carbon all at the same time is enormous, the potential payoffs will also be substantial. By treating harvested CO_2 not as a waste product to be stored—for instance, underground in depleted oil and gas reservoirs—but as a resource, this approach presents both environmental and economic benefits, using the carbon as an income generator rather than as a waste storage cost and opening the door to the possibility that it could pay for itself.

Difficult as the challenges are, Dai said, they're perfect for an institution like ORNL.

"If I can, I'll quote Kennedy, who said we go to the moon not because it's easy, but because it's difficult," Dai said. "That's the reason we really need a holistic approach toward this complex problem."

Making the most of captured carbon

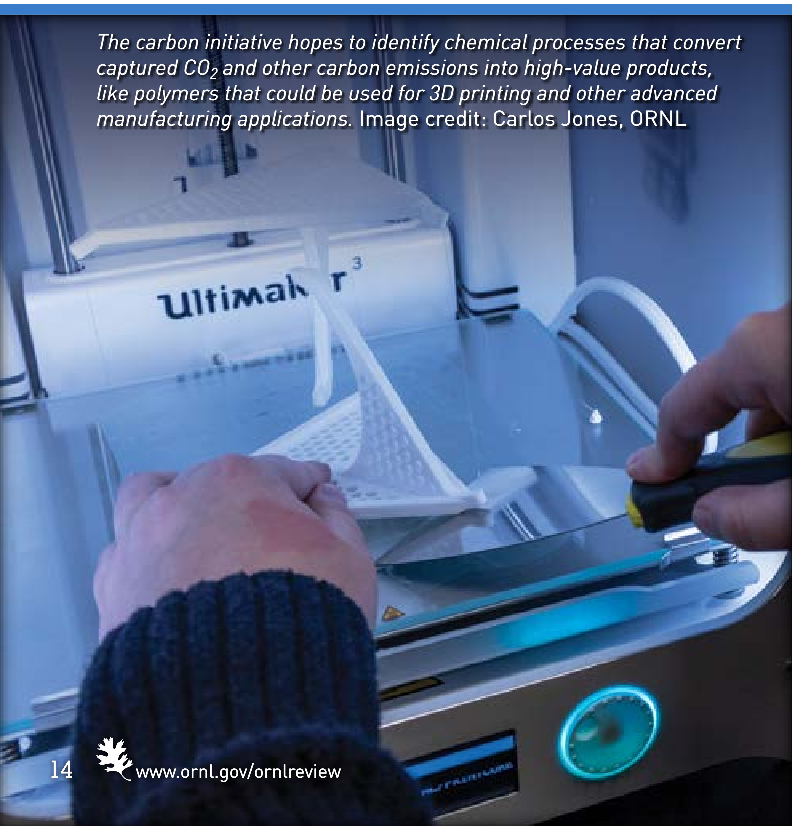
by Jim Pearce
pearcejw@ornl.gov

Historically, one of the major impediments to carbon dioxide mitigation has been cost. So ideally, technological fixes would include ways to recycle excess CO_2 into products that pay for themselves.

To lots of folks, that sounds like a pipe dream—but not to ORNL nanoscientist Rigoberto Advincula, who is heading up the carbon initiative's efforts to identify chemical processes that convert captured CO_2 and other carbon emissions and byproducts into high-value commodities.

Advincula, who leads the Macromolecular Nanoscience Group at the lab's Center for Nanophase Materials Sciences and also serves as Governor's Chair of Advanced and Nanostructured Materials at ORNL and the University of Tennessee, maintains that to balance the carbon cycle, we need to take a holistic approach.

"Sometimes we describe this as creating a 'circular economy,'" Advincula said. "A lot of effort has been put into carbon capture, but this has been basically limited to controlling the carbon footprint of specific industrial processes. Now the challenge is to convert the CO_2 ecosystem into something that benefits society even more. This involves a lot of organic chemistry—essentially the chemistry of carbon."



The carbon initiative hopes to identify chemical processes that convert captured CO_2 and other carbon emissions into high-value products, like polymers that could be used for 3D printing and other advanced manufacturing applications. Image credit: Carlos Jones, ORNL

Modern-day alchemy

"There is a lot of demand for more efficient processes in the coal, oil and natural gas industries where carbon capture technologies have been used to trap 'waste' products, such as methane, for the last 20 or 30 years," Advincula said.

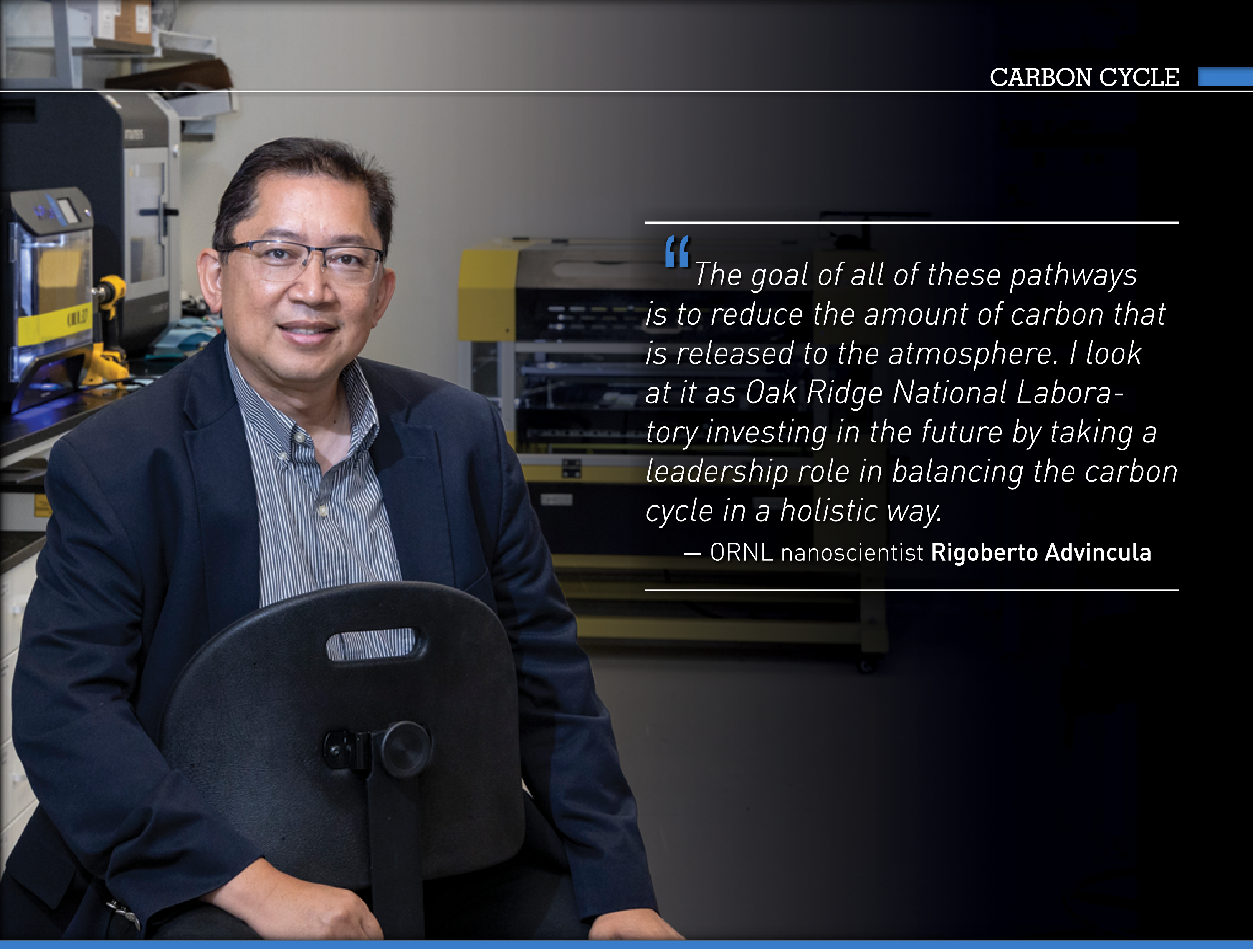
These industries have made considerable progress in turning waste gases like methane into marketable commodities, like organic chemistry "intermediates." Intermediates are chemicals that are used to manufacture a wide range of products—pharmaceuticals, for example—and, importantly, they help to offset the cost of carbon capture.

In the carbon initiative, Advincula's team will improve this waste-to-high-value-product approach by applying more advanced chemistry to produce higher-value materials from CO_2 and other carbon emissions and byproducts.

Many paths, one goal

"These high-value products could include polymers that perform well under extreme conditions, so they could be used to produce advanced composites and other materials used in the aerospace and automotive industries—or for advanced manufacturing applications, such as 3D-printing," Advincula said.

He noted that the construction industry uses a lot of carbon-based thermosets, materials like fiberboard, tiles, and flooring, that make use of carbon fiber and carbon composites.



> *"The goal of all of these pathways is to reduce the amount of carbon that is released to the atmosphere. I look at it as Oak Ridge National Laboratory investing in the future by taking a leadership role in balancing the carbon cycle in a holistic way.*
>
> — ORNL nanoscientist **Rigoberto Advincula**

"The construction industry also relies on plastic for pipes, for different types of roofing material and for a variety of other carbon-based products," Advincula said. "Using advanced chemistry, we will try to create a pathway to make the process of generating these materials from CO_2 and other byproducts of the carbon ecosystem more efficient and more cost-effective."

Another pathway the project will consider is direct carbonization, a process that converts plants, grass or any cellulosic material directly into carbon.

"This approach was popular 20 years ago," Advincula said, "but there are new efficiencies that can be explored, new chemistry, new catalysts that we can use to convert plants directly into building materials."

Advincula will also investigate the possibility of producing high-value materials directly from CO_2 or hydrocarbons like ethane, methane, and propane rather than converting them into intermediate chemicals first. Decreasing the number of steps in the conversion process is another way to reduce the cost of production.

Finally, Advincula's team will use artificial intelligence and machine learning to guide experimental models that will optimize the development of new chemical pathways to streamline the conversion of carbon ecosystem byproducts.

"These tools will enable us to apply data mining to determine which reaction parameters are likely to result in reactions that are faster and more efficient and require less energy," Advincula said. "Unlike previous approaches, the use of AI allows global input—from molecular engineering to process engineering—that will enable new ways of synthesizing complex but practical macromolecular designs."

By developing a range of chemical processes that can convert potentially harmful CO_2 and other carbon emissions into high-value products, the carbon initiative aims to protect the environment while redefining carbon emissions as a valuable, renewable resource.

"The goal of all of these pathways is to reduce the amount of carbon that is released to the atmosphere." Advincula said. "I look at it as Oak Ridge National Laboratory investing in the future by taking a leadership role in balancing the carbon cycle in a holistic way."

Discovery

points the way to more practical superconductors

by Paul Boisvert
boisvertpl@ornl.gov

An ORNL-led international research team may have brought us a step closer to practical room-temperature and room-pressure superconductors with the discovery that hydrogen atoms in a metal hydride material are much more tightly spaced than had been predicted for decades.

Superconductors carry electricity between two points with perfect efficiency and without generating heat. Such a capability at ambient temperatures and pressures would revolutionize a broad range of consumer, medical and industrial applications, paving the way for, among many other things, smaller and faster digital circuits, low-loss power cables, and more powerful and affordable electromagnets for use in magnetic resonance imaging machines, electric motors and generators.

The scientists conducted neutron scattering experiments at ORNL on samples of zirconium vanadium hydride at ambient pressure and at temperatures from −450°F (5 K) to as high as −10°F (250 K)—much higher than the temperatures where superconductivity is expected to occur in these conditions.

Their findings, published in the *Proceedings of the National Academy of Sciences*, detail the first observations of unexpectedly small hydrogen–hydrogen atomic distances in a metal hydride, as small as 1.6 angstroms, compared to the 2.1 angstrom distances predicted for these metals.

This interatomic arrangement is promising because the hydrogen contained in metals affects their electronic properties. Other materials with similar hydrogen arrangements have been found to start superconducting, but only at extremely high pressures.

"Some high-temperature superconductors start superconducting at about 8.0°F, but unfortunately this requires enormous pressures—as high as 22 million pounds per square inch," said Timmy Ramirez-Cuesta of ORNL's Neutron Scattering Division.

Russell J. Hemley, professor and Distinguished Chair in the Natural Sciences at the University of Illinois at Chicago, added, "For decades, a holy grail for scientists has been to find or make a material that superconducts at room temperature *and* atmospheric pressure, which would allow engineers to design it into conventional electrical systems and devices."

> "ORNL is the only place in the world that boasts both a world-leading neutron source and one of the world's fastest supercomputers.
>
> — **Timmy Ramirez-Cuesta** of ORNL's Neutron Scattering Division

The researchers had probed the hydrogen interactions in the well-studied metal hydride with high-resolution, inelastic neutron vibrational spectroscopy on the VISION beamline at the Spallation Neutron Source at ORNL. Neutrons can easily penetrate metals, and they scatter strongly from the nuclei of hydrogen atoms, which make them ideal for finding the hydrogen inside the metal hydride material. However, the resulting spectral signal, including a prominent peak at around 50 millielectronvolts, did not agree with what computer models predicted.

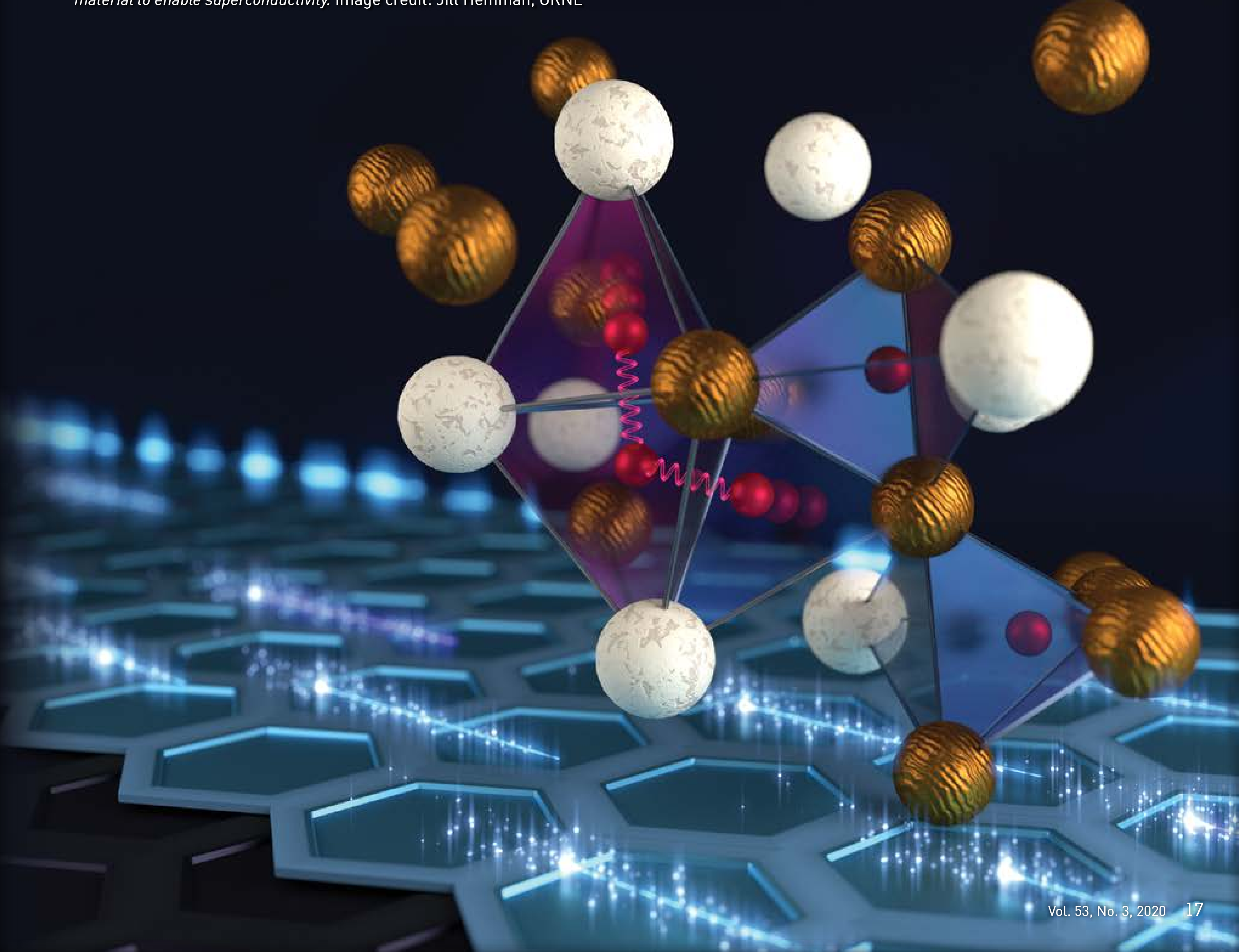
A breakthrough in their understanding occurred after the team began working with the Oak Ridge Leadership Computing Facility to develop a strategy for evaluating the data. The OLCF at the time was home to Titan, one of the world's fastest supercomputers.

"ORNL is the only place in the world that boasts both a world-leading neutron source and one of the world's fastest supercomputers," said Ramirez-Cuesta. "Combining the capabilities of these facilities allowed us to compile the neutron spectroscopy data and devise a way to calculate the origin of the anomalous signal we encountered. It took an ensemble of 3,200 individual simulations, a massive task that occupied around 17 percent of Titan's immense processing capacity for nearly a week—something a conventional computer would have required 10 to 20 years to do."

These computer simulations, along with additional experiments ruling out alternative explanations, proved conclusively that the unexpected spectral intensity occurs only when distances between hydrogen atoms are closer than 2.0 angstroms, which had never been observed in a metal hydride at ambient pressure and temperature.

In future experiments, the researchers plan to add more hydrogen to zirconium vanadium hydride at various pressures to evaluate the material's potential for electrical conductivity. ORNL's latest supercomputer, Summit—currently the nation's fastest—could provide the additional computing power that will be required to analyze these new experiments.

Metal hydride structure with surprisingly small distances between hydrogen atoms (in red) at near-ambient conditions. These smaller spacings might allow packing significantly more hydrogen into the material to enable superconductivity. Image credit: Jill Hemman, ORNL



New synthetic polymers

rival their protein counterparts

by Paul Boisvert
boisvertpl@ornl.gov

Biological membranes, including the walls of most types of living cells, consist primarily of a double layer of lipids—a lipid bilayer—that forms the structure, and a variety of embedded and attached proteins with highly specialized functions. Many of these proteins are involved in rapidly and selectively transporting materials in and out of the cell.

Artificial membranes, which mimic their natural counterparts, have been used for small- and large-scale industrial processes since the mid-20th century, yet their inefficiency makes some of these processes slow and expensive. Scientists have long sought to develop synthetic membranes that match the selectivity and high-speed transport offered by their natural counterparts.

Now researchers led by a team from the University of California, Berkeley, and making use of ORNL's High Flux Isotope Reactor have reported the development of a novel polymer that is as effective as natural proteins in transporting protons through a membrane. Their work appears in the journal *Nature*.

> *"We inserted our new polymers into lipid bilayers, and they transported protons just as well as natural proteins.*
> — University of California, Berkeley, Professor **Ting Xu**

This major milestone has the potential to transform a wide range of technologies, making batteries and water purification systems more efficient and less expensive, for instance, and lowering the cost of producing biofuels and pharmaceuticals.

"We inserted our new polymers into lipid bilayers, and they transported protons just as well as natural proteins," said Ting Xu, a professor at UC Berkeley and faculty scientist for the Materials Sciences Division at Lawrence Berkeley National Laboratory.

"The polymers are very difficult to image and study because of the limited contrast between their density and that of lipids," she said. "So we enhanced the contrast by selectively deuterating the lipids in the samples—meaning we replaced some of their hydrogen atoms with deuterium atoms—which neutrons are especially good at differentiating from hydrogen atoms. That allowed us to use neutron scattering at Oak Ridge to better 'see' the size and shape of the individual polymers."

Working at HFIR, the researchers used the general purpose small-angle neutron scattering, or GP-SANS, beamline to conduct their experiments. SANS is a nondestructive experimental technique for probing all sorts of complex materials—including polymers and biological structures—which leverages the power of the differences in how neutrons interact with different elements and their isotopes, particularly hydrogen and deuterium.

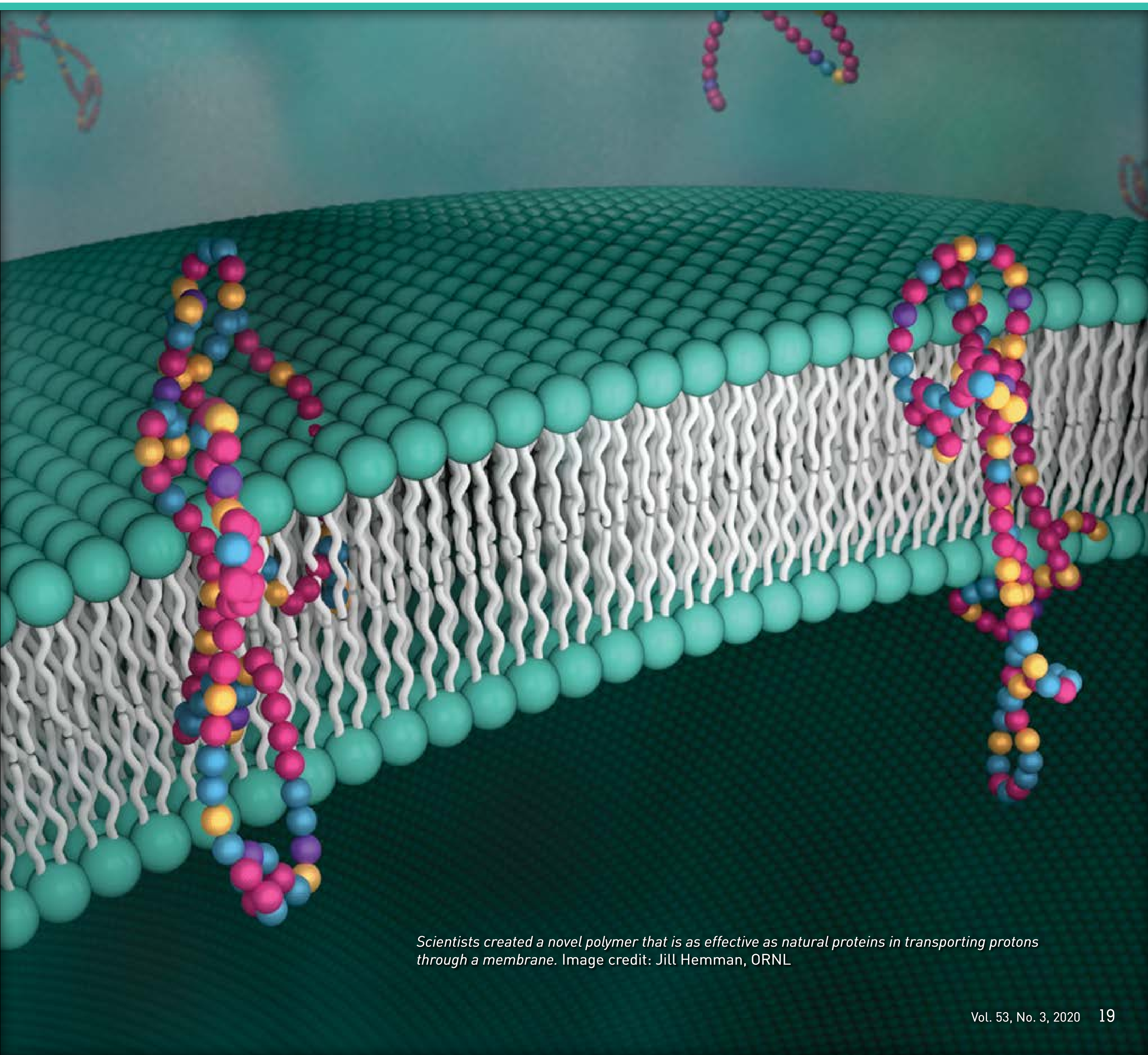
"The GP-SANS instrument enabled the team to determine the polymers were compact structures that were randomly dispersed within the membrane—as opposed to clumped together," said William T. Heller, who supports instrumentation. "We chose the GP-SANS instrument because it is ideal for the polymer's size, and its intense beam is excellent for studying samples that do not scatter neutrons strongly."

Xu and her collaborators said that four monomers, the main components of the new polymer, can be grouped in different ways to produce functional protein mimics.

"It should be possible to break the polymer chain into building blocks, like Lego pieces," she said. "The pieces can then be put back together in specific ways to recreate the functions of natural proteins."

Xu and her team are developing a library of polymers that are similar in sequence to provide more flexibility in assembly. The researchers plan to create these polymers, which are truly protein-like in their functions, after determining the rules of how the polymers work together.

"What makes our new technique so promising is that it's scalable, and the knowledge to do this is readily available," Xu said. "Considering the vast number of monomers available and the recent advances in polymer chemistry, the possibilities of marrying the synthetic and biological fields are almost unlimited."



Scientists created a novel polymer that is as effective as natural proteins in transporting protons through a membrane. Image credit: Jill Hemman, ORNL

Record-breaking

supercomputer simulations aid COVID-19 research

by Rachel Harken
harkenrm@ornl.gov

Before COVID-19 was declared a pandemic by the World Health Organization on March 11, 2020, researchers at ORNL were already using the nation's most powerful supercomputer, the lab's Summit system, to study the novel SARS-CoV-2 virus.

> "Summit is a general-purpose supercomputer and, therefore, it can attack a multitude of scientific problems. We are very cognizant of the fact that it's ultimately the U.S. taxpayer who paid for Summit, and we believe that everybody would think that this is a valid and important use of this important national resource.
>
> — Oak Ridge Leadership Computing Facility Director of Science **Bronson Messer**

Now, 21 different COVID-19 projects are running on Summit, involving everything from drug targets to pandemic models to gene expression analyses, and some of them are getting big results. The move to allocate some of the lab's supercomputing hours to COVID-19 was, in part, a result of the creation of the COVID-19 High-Performance Computing Consortium, an international public–private collaboration of government, university and industry leaders providing access to HPC systems to support COVID-19 research.

The first team to perform COVID-19 work on Summit was led by Jeremy Smith, director of the University of Tennessee/ORNL Center for Molecular Biophysics and Governor's Chair for Molecular Biophysics at the University of Tennessee, Knoxville. His team simulated different compounds docking to the virus' spike protein to determine if any of the compounds might prevent it from sticking to human cells.

Initially, the researchers screened more than 8,000 drug compounds—including medications and natural compounds—and identified 77 that were shown by the simulations to bind to regions of the spike that are important for entry into the human cell. This paved the way for the team to complete a screening of 1.5 billion chemical compounds in 24 hours on Summit—the largest drug screening study ever undertaken on a supercomputer. The team simulated the compounds binding to the SARS-CoV-2 main protease, the enzyme that enables the virus to reproduce.

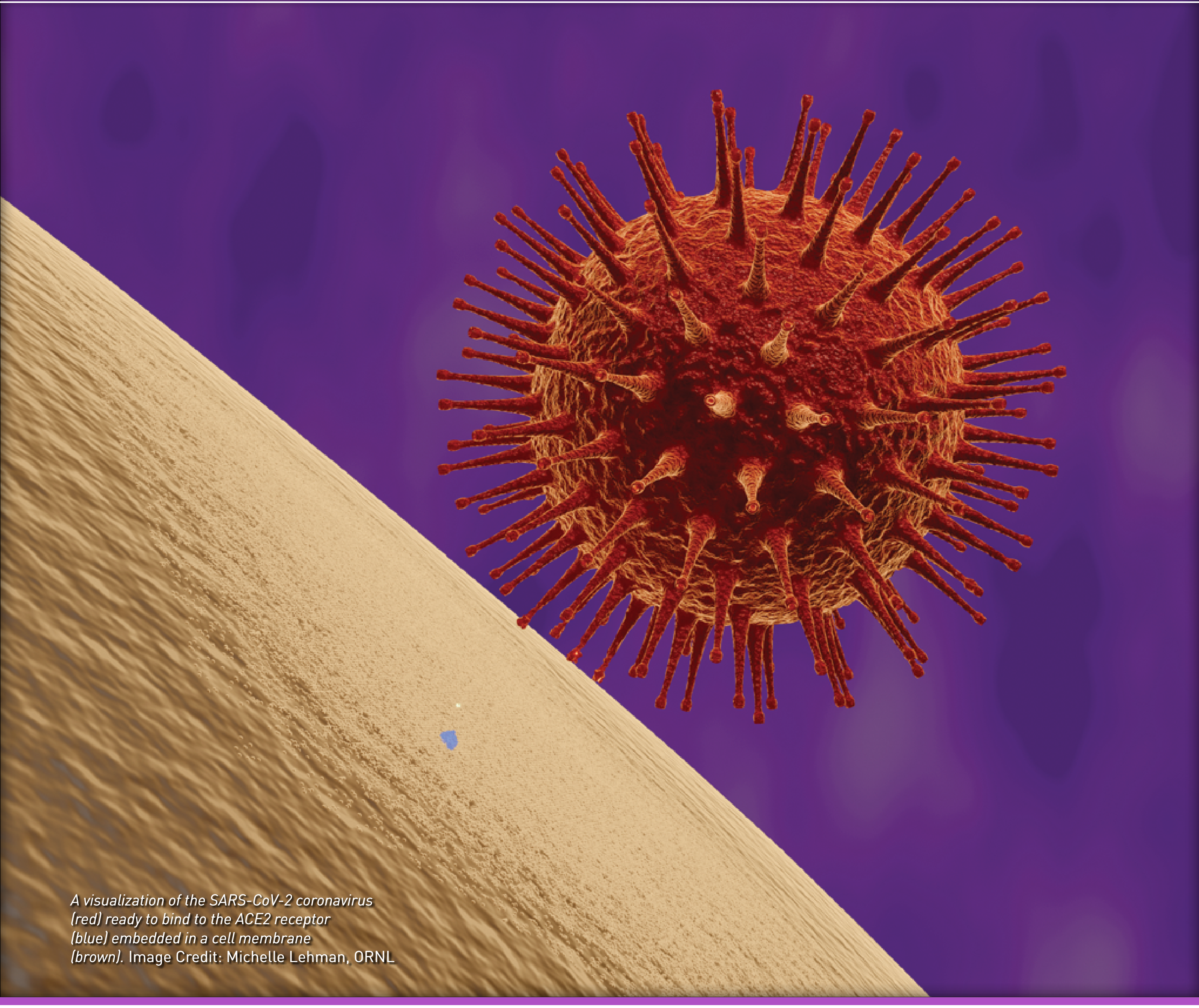
"We broke a world record on the supercomputer," Smith said.

After the first study, the team reached out to Professor Colleen Jonsson at the University of Tennessee Health Sciences Center in Memphis, Tennessee, to test possible drugs targeting the spike protein. Her team hopes to be running animal tests for a variety of possible COVID-19 drugs by the end of the year.

Other teams have also gained steam using Summit for COVID-19 research in recent months.

A team led by ORNL computational biologist Dan Jacobson used Summit to compare samples of lung fluid cells from COVID-19 patients with control patients to look at gene expression and co-expression patterns in the cells. Based on the findings, the researchers believe one of the body's systems responsible for lowering blood pressure—the bradykinin system—may explain the runaway symptoms produced by the body's response to SARS-CoV-2.

At least 10 existing drugs are known to act on the specific pathways Jacobson's team studied, but large-scale clinical trials



A visualization of the SARS-CoV-2 coronavirus (red) ready to bind to the ACE2 receptor (blue) embedded in a cell membrane (brown). Image Credit: Michelle Lehman, ORNL

are needed to determine whether they might be effective at treating COVID-19.

"If we can block this pathogenesis in severe patients, we can keep the human response from going overboard and give their immune system time to fight off the virus so they can recover," Jacobson said.

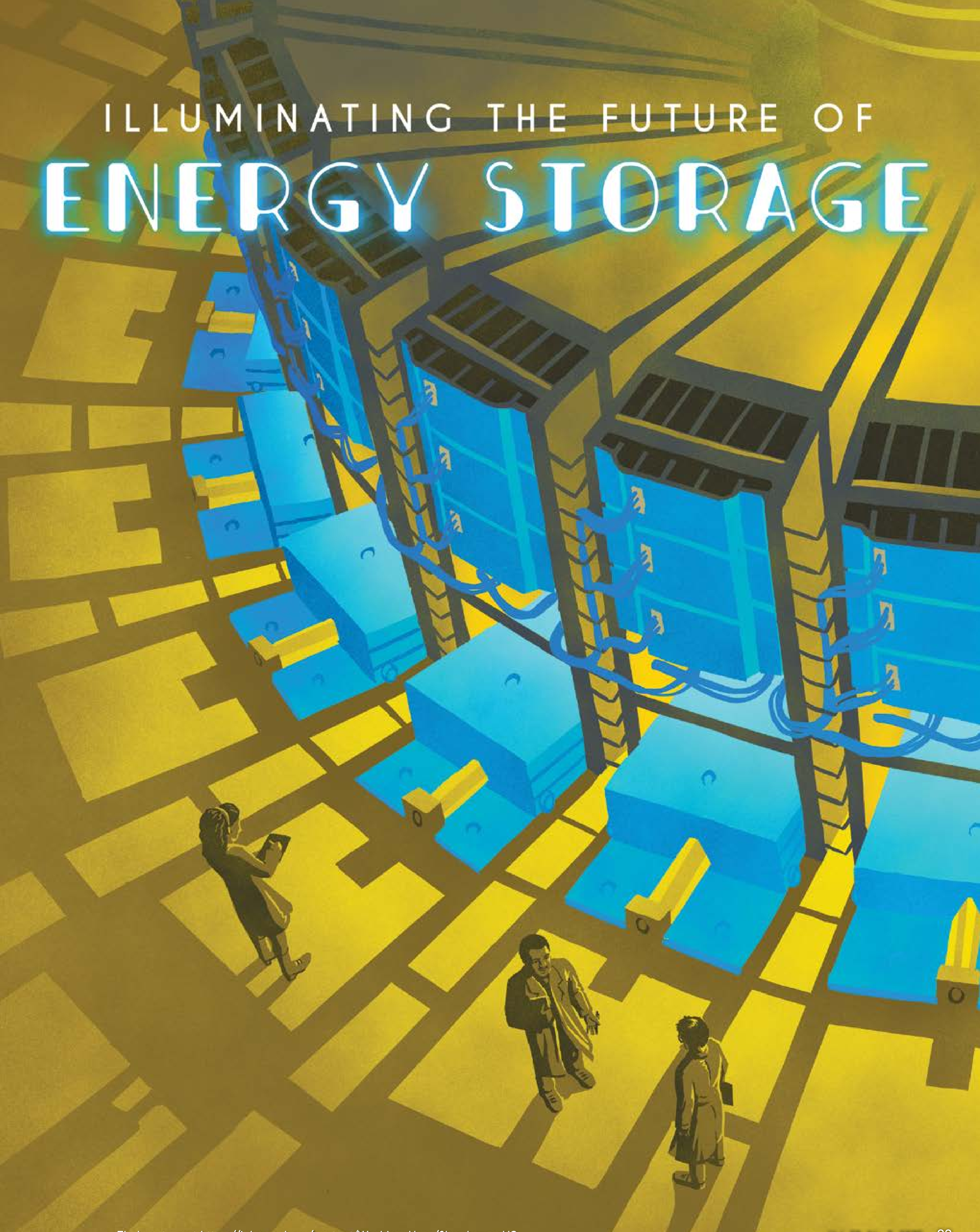
Jennifer Diaz of the Icahn School of Medicine at Mount Sinai and team are also studying gene expression patterns related to COVID-19, but instead of studying data from lung cells, they're predicting gene expression patterns for more than 700,000 combinations of existing drugs using a machine learning classifier on Summit. Diaz's team has identified FDA-approved drugs that are already being studied to treat COVID-19 as well as novel drugs that may have a synergistic effect when combined.

The transition to COVID-19 work on Summit reveals the versatility of the machine as well as the scientists working on the system.

"Summit is a general-purpose supercomputer and, therefore, it can attack a multitude of scientific problems," said Bronson Messer, director of science at the Oak Ridge Leadership Computing Facility. "We are very cognizant of the fact that it's ultimately the U.S. taxpayer who paid for Summit, and we believe that everybody would think that this is a valid and important use of this important national resource."

ORNL research includes funding from the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on response to COVID-19, with funding provided by the Coronavirus CARES Act.

Find posters at https://jobs.ornl.gov/content/Working-Here/?locale=en_US



Find posters at https://jobs.ornl.gov/content/Working-Here/?locale=en_US

Quantum technologies go the distance

by Elizabeth Rosenthal
rosenthalec@ornl.gov

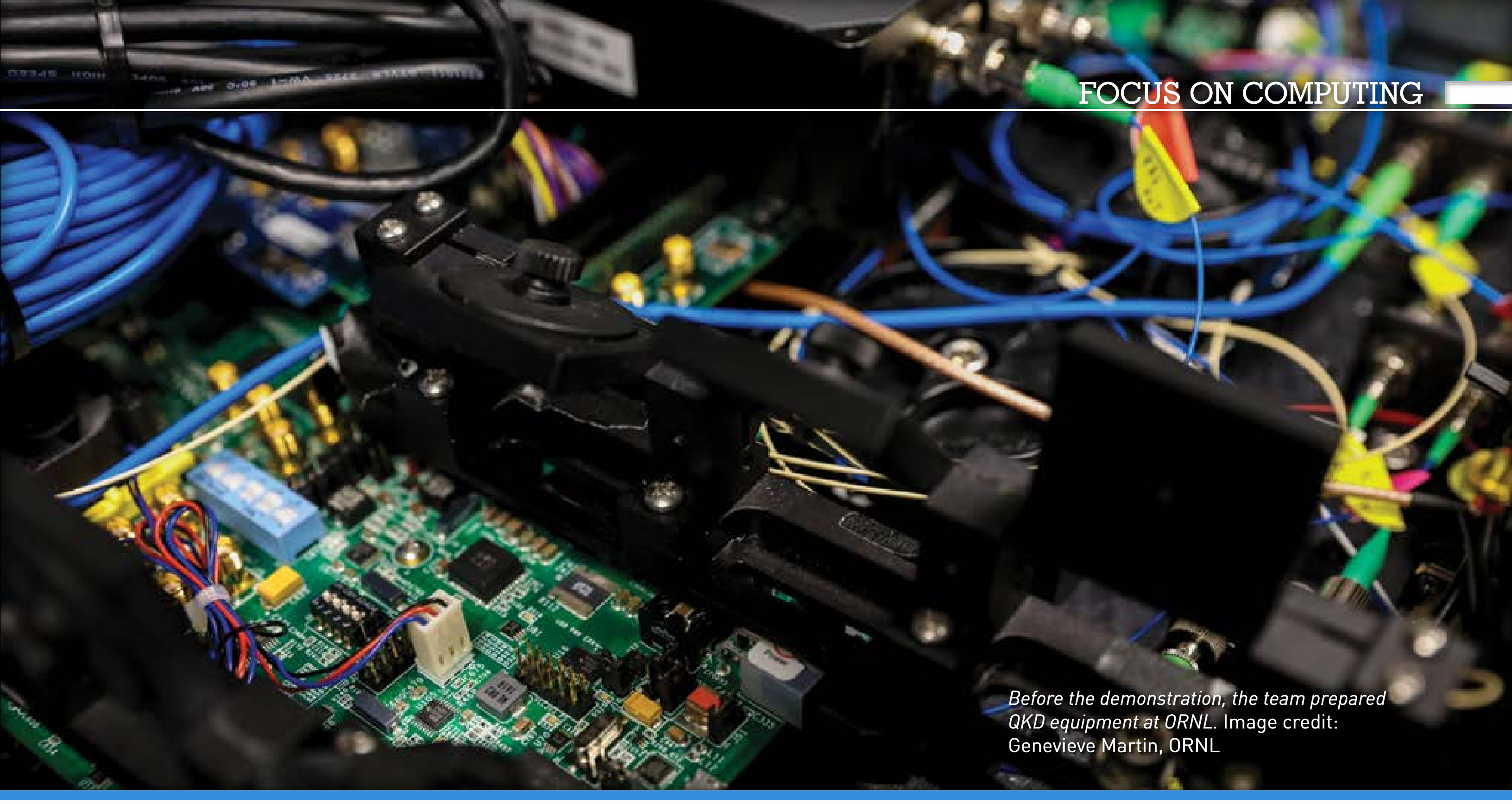
A team from ORNL and Los Alamos National Laboratory has greatly increased the range covered by quantum-based technologies that could improve the cybersecurity, longevity and efficiency of the nation's power grid.

Specifically, the team demonstrated quantum key distribution, or QKD, systems that use quantum mechanics to authenticate data and encrypt messages with a secret key. Using private encryption methods, the key securely transmits locked information from one QKD system to another through a trusted node that is resistant to cyberattacks.

"This technology relies not on the mathematical laws that govern modern computer security but on the physical laws of quantum mechanics that do not change over time," said Raymond Newell, who leads LANL's quantum communications team. "As a result, we can make security assurances that will remain true indefinitely because they do not rely on assumptions."

The demonstration was the second such event hosted by EPB, a utility and telecommunications company serving Chattanooga, Tennessee. Last year, ORNL, LANL and EPB used an isolated portion of EPB's fiber-optic network to demonstrate that QKD systems can communicate even when they have different hardware

ORNL quantum researchers, from left, Brian Williams, Phil Evans and Nicholas Peters work on the QKD system developed with Qubitekk. Image credit: Genevieve Martin, ORNL



Before the demonstration, the team prepared QKD equipment at ORNL. Image credit: Genevieve Martin, ORNL

and software components, an important step toward ensuring the compatibility of equipment from various vendors.

This year, the team placed QKD systems developed by ORNL, LANL and Qubitekk, a QKD developer and manufacturer, in electrical substations connected by the portion of EPB's fiber-optic network set aside for testing. The substations served as pitstops that allowed each system to pass the key to the next system.

Severe distance limitations previously prevented QKD from becoming a viable addition to existing grid management techniques, but the team proved that three distinct systems can complete a real-world relay of quantum keys across the city.

"Successfully demonstrating QKD performance in a real environment helps establish the feasibility of this technology for protecting critical energy delivery infrastructure," said Nicholas Peters, who leads ORNL's Quantum Information Science Group.

Storing the QKD systems in substations—boxes surrounded by buildings, cameras, fences and other security measures—provided cyber and physical protection.

"QKD is unique because it can detect the presence of any eavesdropper who attempts to intercept and copy information," said Phil Evans of the Quantum Information Science Group. "These interceptions show up as errors, and we throw them away before they can leak any key information."

The QKD approach also allows multiple substations to exist on the quantum network, enabling the control center to securely issue critical instructions to all of them simultaneously.

"With this technology, utilities get better cybersecurity without introducing administrative headaches. It is a set-and-forget solution that simplifies cybersecurity operations for utilities," said Duncan Earl, president and chief technology officer of Qubitekk.

QKD systems integrated into the grid could improve cybersecurity, efficiency and durability by remaining functional and secure for decades along with the physical infrastructure. With one of the most advanced smart grids in the country, EPB has become a pioneer in grid research through longstanding partnerships and novel demonstrations.

"We are proud of our partnership with DOE, ORNL and LANL and that EPB could host this quantum-based security field test for this simulation," said Steve Morrison, EPB's director of information security. "These smart grid demonstrations help us develop promising technology to help protect America's electric grid from cyberattacks."

ORNL and LANL researchers continue to develop quantum technologies—some of which are commercially licensed, others in the early stages of testing—and both laboratories plan to continue collaborating with EPB.

The team hopes to deploy more QKD resources to the national grid system to test these same advancements on a much larger scale.

> *"QKD is unique because it can detect the presence of any eavesdropper who attempts to intercept and copy information. These interceptions show up as errors, and we throw them away before they can leak any key information.*
>
> — ORNL QIS Group's **Phil Evans**

New device will test materials for fusion reactors

by Adriana Ghiozzi
ornlreview@ornl.gov

Temperatures hotter than the center of the sun. Magnetic fields hundreds of thousands of times stronger than the Earth's. Neutrons energetic enough to change the structure of a material. These are not the conditions on a faraway planet; they're the normal demands inside a fusion reactor.

This extreme environment of ionized gases known as plasmas poses a challenge for scientists and engineers nearly as daunting as that of producing fusion itself, namely, creating materials tough enough to withstand high-power plasma conditions over long periods of time.

"If you want to have fusion power, and eventually a fusion reactor that runs most of the time, that will have a big impact on your material requirements," said Juergen Rapp of ORNL's Material Plasma Exposure eXperiment, or MPEX. "You will chew through material with steady-state operation over many years.

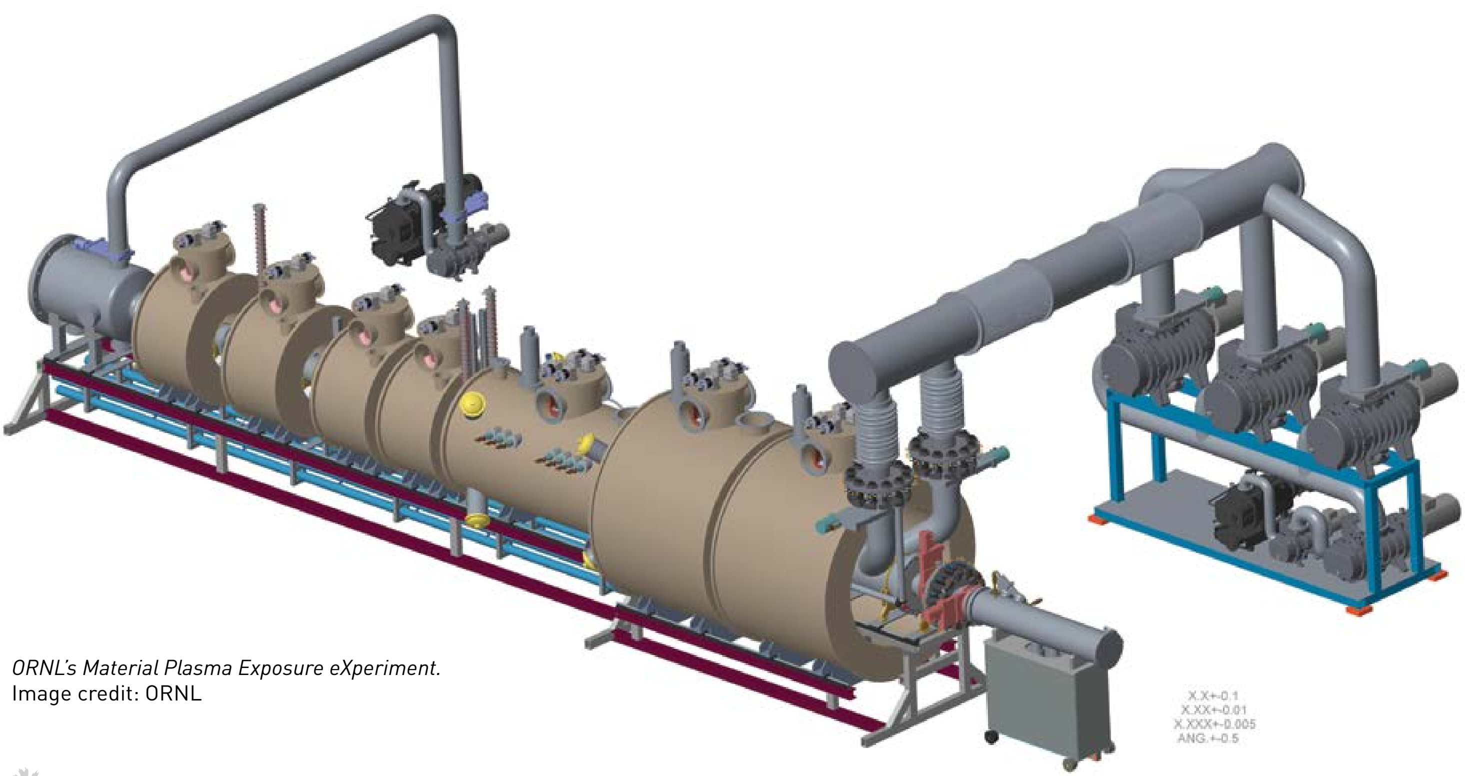
"For a long time, physicists studied the effect of the materials on the plasma, but looking forward, we have to study the effect of the harsh conditions of a burning plasma on the materials."

With that goal in mind, researchers in the lab's Fusion and Fission Energy and Science Directorate are preparing a design for MPEX, a next-generation linear plasma device that will support study of the long-term interactions between plasmas and the components of future fusion reactors.

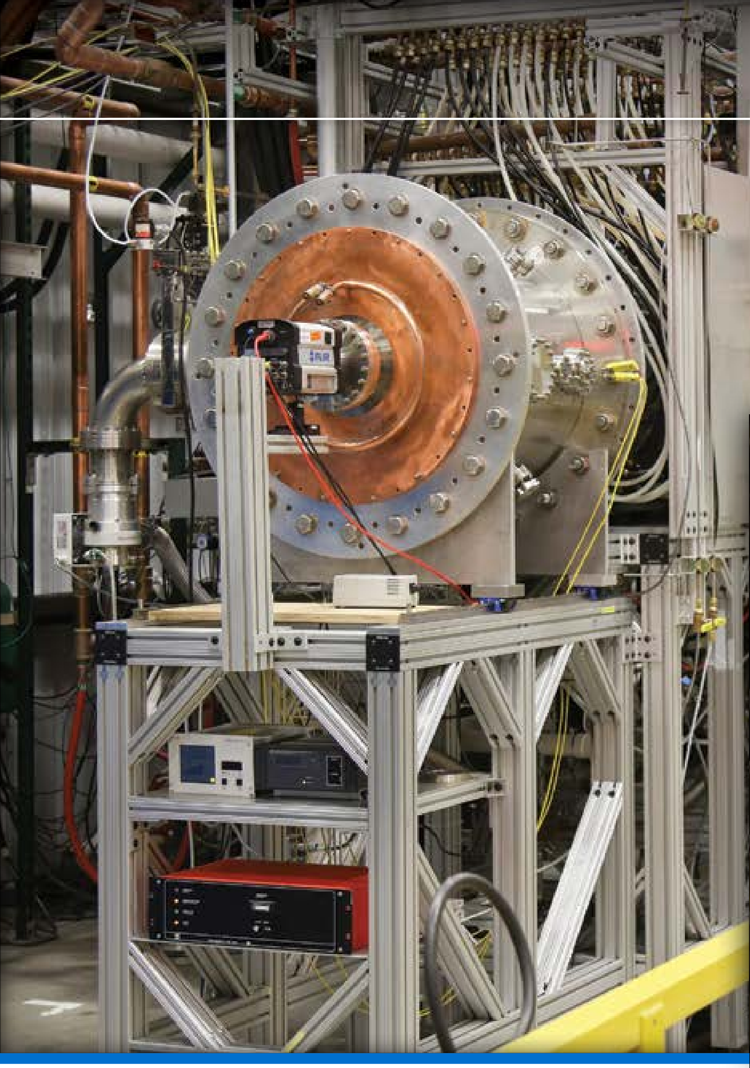
ORNL has the largest materials program within DOE's Office of Science. It also hosts US ITER, the United States' contribution to the international ITER project, which is now under construction in France. ITER is the world's largest fusion experiment and will demonstrate a 500-megawatt burning plasma.

Achieving commercial-scale fusion energy is considered one of the greatest engineering challenges of the 21st century.

"Our work on plasma–material interaction with MPEX is the bridge between burning plasma physics and the materials science knowledge we have obtained from small material samples," Rapp said.



ORNL's Material Plasma Exposure eXperiment.
Image credit: ORNL



The proto-MPEX explores plasma–material interactions under conditions similar to those on the surface of the sun. Image credit: Jason Richards, ORNL

MPEX scientist Juergen Rapp.
Image credit: Genevieve Martin, ORNL

In MPEX, a high-power radio-wave source will create sizeable, high-density, high-temperature plasmas that will replicate the conditions of a fusion reactor.

> "For a long time, physicists studied the effect of the materials on the plasma, but looking forward, we have to study the effect of the harsh conditions of a burning plasma on the materials.
>
> — ORNL Material Plasma Exposure eXperiment scientist **Juergen Rapp**

"MPEX is expected to exceed the conditions of any current materials testing device," said Phil Ferguson, the MPEX project director. "Using a prior neutron source, it can expose samples to plasmas that replicate radiation exposure conditions relevant for a prototype fusion reactor."

Scientists will also take advantage of ORNL's High Flux Isotope Reactor. HFIR will expose materials to neutron fluxes comparable to those of a fusion reactor before the samples are placed into MPEX. The two devices will together provide a complete picture of the combined effect that irradiation, high heat loads, and large magnetic fields have on potential reactor component materials.

"At ORNL, we're familiar with irradiated materials, thanks to our nuclear history. We are designing for that from the beginning," said Ferguson.

As the fusion community begins to look past experimental devices like ITER and toward commercially viable fusion power, MPEX will answer some crucial questions. A recent US fusion community report to the DOE Fusion Energy Sciences Advisory Committee emphasized the importance of focusing on both prototype reactor development and essential fusion technologies, such as reactor materials.

After coming online in the 2020s, MPEX will enable the design of new materials and ultimately inform materials choices for prototype and eventually industrial fusion reactors.

"We have nearly a 70-year history in fusion energy research and development at ORNL," said ORNL Associate Laboratory Director Alan Icenhour. "Because of that extensive foundation and the current collection of diverse fusion expertise, this is the ideal location for discovering how to advance fusion materials beyond what we have available today."

Nuclear consortium

leaves industry with advanced simulation tool

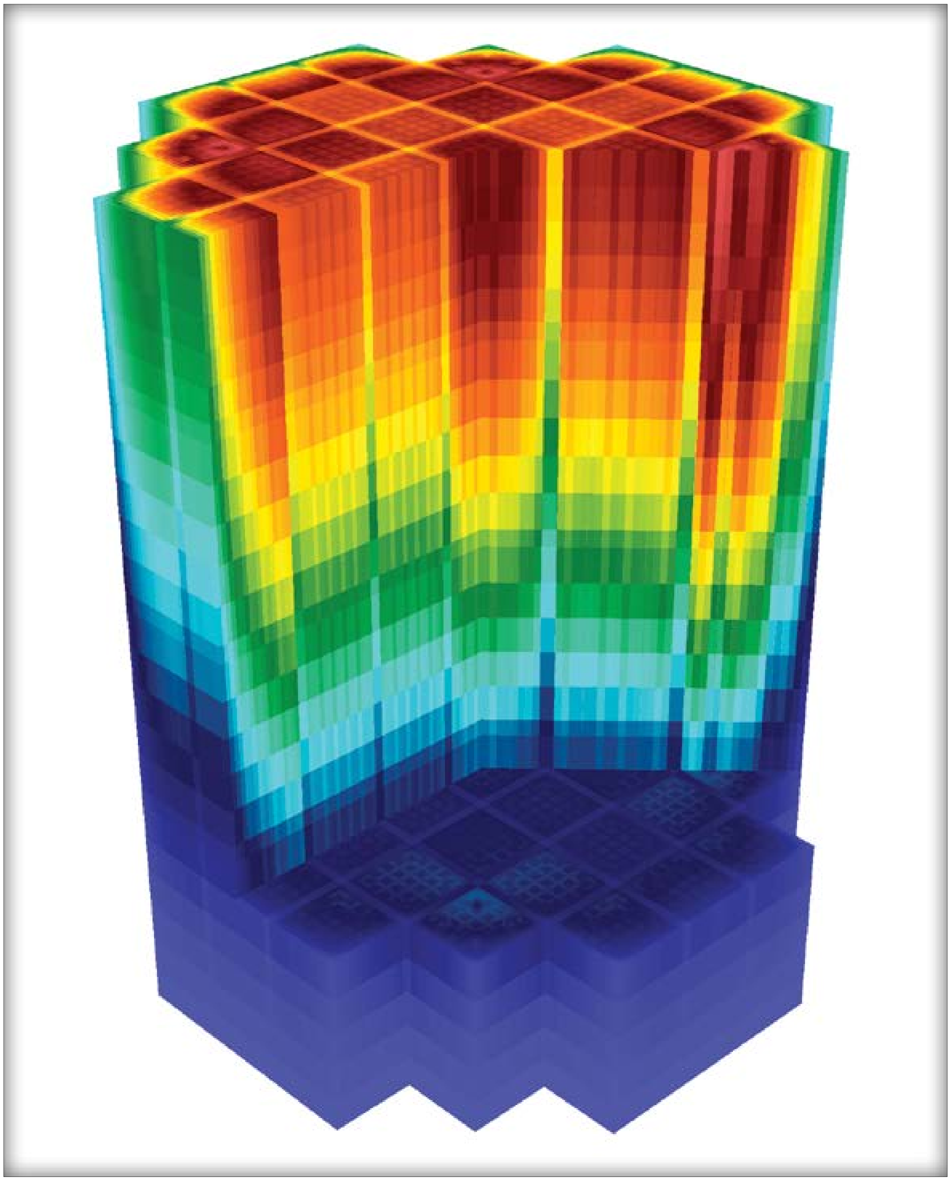
by Kristi Nelson Bumpus
bumpuskl@ornl.gov

Ten years ago, the Consortium for Advanced Simulation of Light Water Reactors became DOE's first Energy Innovation Hub. Its mission was to make nuclear reactors more efficient and ultimately extend the life of the nation's aging reactor fleet.

In that time, the consortium—a national collaboration of scientists and engineers from government, academia and industry—identified six key challenges. It ultimately produced a suite of software—the Virtual Environment for Reactor Applications, or VERA—that can predict the behavior of nuclear reactor cores with stunning accuracy, down to a single fuel rod.

"We developed a virtual simulation technology that could pretty convincingly tackle the problem, that could simulate the physical phenomena and give us engineering insight as to why these problems were happening and how to ameliorate them," said Doug Kothe, CASL director for its first five years. "We put the entire reactor into a computer."

Now, with CASL wrapped up at the end of June, the program is turning that technology over to industry for its own use.



VERA's tools allow a virtual window inside a nuclear reactor core, down to a molecular level.
Image credit: ORNL

The CASL team poses after receiving DOE's R&D 100 award in 2016. The award recognizes the most promising new products, processes, materials and software developed throughout the world and introduced to the market the previous year. Image credit: Jason Richards, ORNL

Current director Dave Kropaczek said he expects more than a dozen companies to procure licenses to use VERA. More than 400 individuals are licensed to use it.

"The Electric Power Research Institute, one of our core CASL industry partners, already has the right to use VERA to perform services for its member utilities," Kropaczek said. "Our partners in the nuclear industry wanted software that was proven and useful, and that's exactly what we've produced."

> *"We developed a virtual simulation technology that could pretty convincingly tackle the problem, that could simulate the physical phenomena and give us engineering insight as to why these problems were happening and how to ameliorate them. We put the entire reactor into a computer.*
>
> — Former CASL Director **Doug Kothe**

The VERA software suite is a collection of interfacing codes that can simulate reactor core behavior from the large scale down to the molecular scale. It promotes improved performance and longer lifetimes for the current reactor fleet by providing advanced modeling and simulation capabilities to help address several challenges.

VERA can predict departure from nucleate boiling, for instance, which occurs when steam bubbles no longer break away from a rod, instead forming a vapor layer that interferes with the transfer of heat. In addition, it can model the growth of corrosion deposits on fuel rods, the ongoing integrity of both fuel pellets and cladding during normal operation and postulated accident scenarios, and the performance of reactor parts when exposed to high temperatures and radiation.

CASL's new VERA Users Group will provide training, ongoing support and access to DOE's high-performance computing resources to perform large-scale simulations.

Last year, CASL ensured the VERA software quality assurance program is in Nuclear Quality Assurance-1 compliance in preparation for widespread industry use. NQA-1 compliance, the gold standard for the nuclear industry, signifies extensive efforts in the areas of procedures, training and software control.

Kothe said CASL demonstrated the value of the DOE Energy Innovation Hub model.

"If you have an important national problem and enough stable funding to go after that problem for multiple years, with multiple institutions, then you're going to attract the best and the brightest to solve that problem," Kothe said.

Remote-controlled

system can repair radioactive canisters

by Kristi Nelson Bumpus
bumpuskl@ornl.gov

A team of ORNL researchers has developed a device for remotely repairing stainless-steel containers of spent nuclear fuel and high-level radioactive waste—without moving or even touching them.

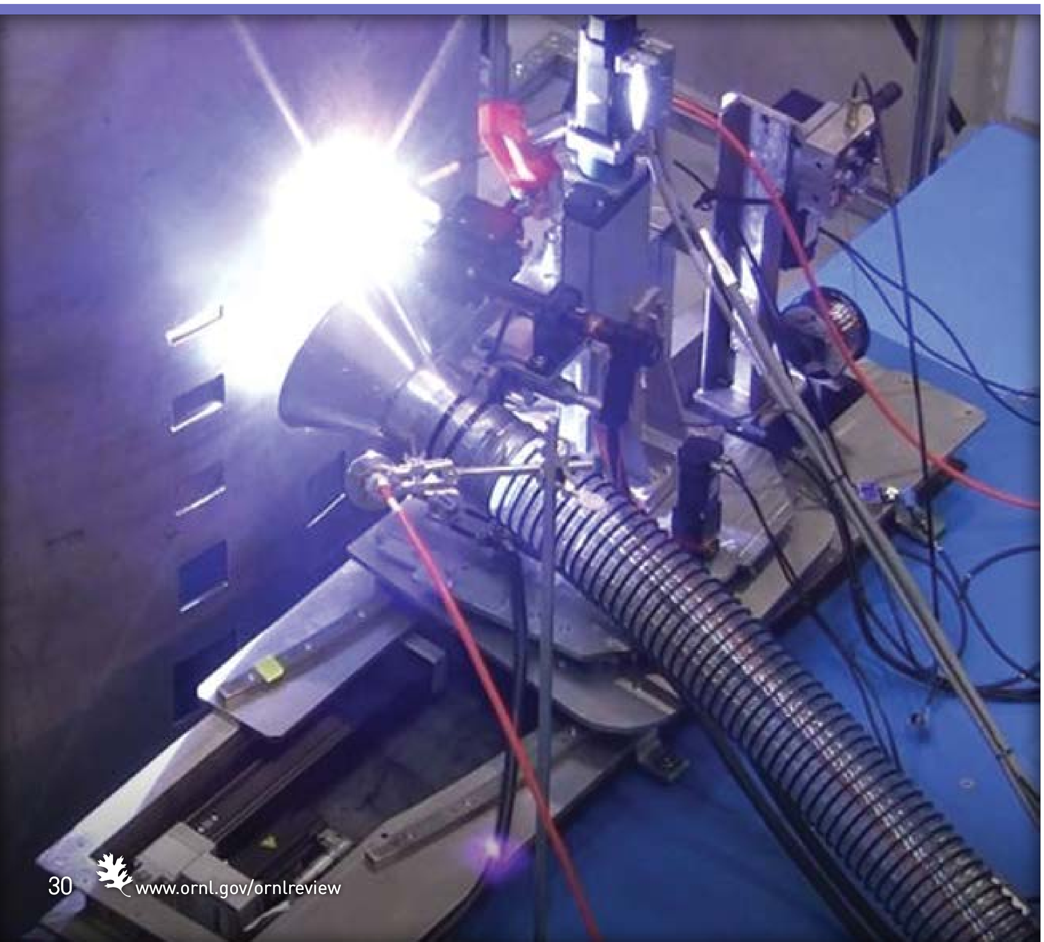
The team, led by Stylianos Chatzidakis of the Nuclear Energy and Fuel Cycle Division, successfully demonstrated a prototype module to remotely repair the welded containers, which under certain conditions may be vulnerable to corrosion and eventual cracking. High radiation levels and limited space prevent hands-on repairs, and the large number of canisters—about 3,200 currently and likely 10,000 or more by 2050—mandates a largely automated repair method.

Specifically for welding in high-radiation zones

The first-of-its-kind Versatile Remediation Module, which ORNL began designing and building in 2017, is computer controlled. It was built specifically for applications where hands-on repair is not possible, said Chatzidakis, whose expertise is in developing novel ways to ensure safe and secure storage of spent nuclear fuel in containers—a task made more complex because the containers shouldn't be reopened once sealed.

"Currently, we expect spent nuclear fuel to remain in dry storage for much longer periods of time than initially anticipated—up to 60 years or more, in some cases," Chatzidakis said. "Safe and effective management of our spent fuel inventory is an important aspect of nuclear energy for today and the future."

The VRM, built largely from off-the-shelf components, uses a real-time controller connected to a workstation by standard Ethernet. Having the controller near the VRM minimizes cable lengths while allowing the operator to be remote.



This snapshot of the Versatile Remediation Module shows a stainless-steel canister with "pockets" on the surface being welded by computer control. Each pocket was filled with five passes of overlay weld material. Image credit: ORNL

The module's design uses an air-cooled gas tungsten arc welding torch to eliminate the possibility that the repair could induce later corrosion, as well as instrumentation to measure the preprogrammed voltage and keep it consistent during welding. The filler wire used for the weld is guided into place through a wire feeder assembly, and during the weld ultra-high-purity argon forms a shield for the wire and feeder assembly, to reduce contaminations and unwanted chemical reactions.

The initial demonstration of a complete remote repair weld on a full-scale stainless-steel canister was done from 100 feet away, with no direct line of sight.

"The success of this effort demonstrates the unique capabilities of ORNL in the fields of nuclear and mechanical engineering and exemplifies how these capabilities can be used to solve actual real-world challenges," said Rose Montgomery of the Nuclear Energy and Fuel Cycle Division.

Other applications likely

The multidivision VRM team has submitted a paper to the journal *Nuclear Technology*, and a provisional patent application has been approved for the system.

The team believes the scope of the VMR will go far beyond this specific task. Because it's designed to accommodate even more remediation techniques, many of VMR's features and concepts could be used for other remote nuclear or nonnuclear applications. Ultimately, it could serve as a hub to facilitate and enhance further development of new remediation technologies by national laboratories, universities and industry.

"With an understanding of radiation interactions with materials, the VRM was able to be built with mostly off-the-shelf equipment, allowing it to be fabricated quickly at low cost while maintaining a robust and rugged design," said Dominic Giuliano, lead VRM engineer.

"The VRM is a clear example of what design expertise and a fundamental understanding of radiation can achieve."

Dominic Giuliano of ORNL's Fusion Energy Division stands with an empty canister used to demonstrate an ORNL-built remote module that uses computer controls to weld stainless-steel canisters containing spent nuclear fuel. Image credit: ORNL

> *"The success of this effort demonstrates the unique capabilities of ORNL in the fields of nuclear and mechanical engineering and exemplifies how these capabilities can be used to solve actual real-world challenges.*
>
> — **Rose Montgomery** of the Nuclear Energy and Fuel Cycle Division

Curved crystals

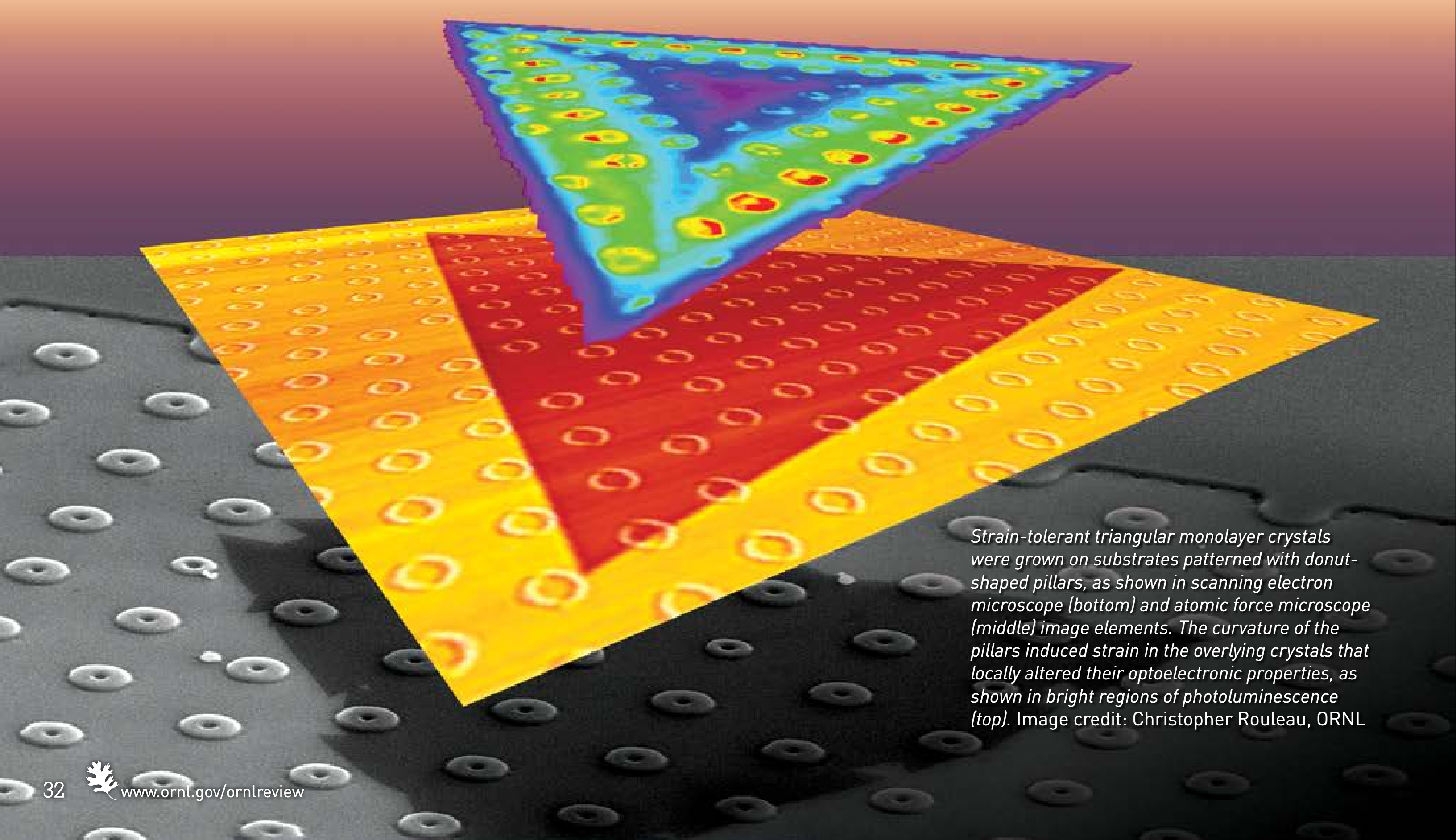
are promising for quantum devices

by Dawn Levy
levyd@ornl.gov

An ORNL-led team has found a strategy for advancing quantum information processing.

When an atomically thin 2D crystal is grown over an orderly arrangement of 3D shapes placed on a substrate, the curvatures of the objects stretch and strain the crystal. The researchers explored how to engineer that strain to produce "hot spots" in the array that can each emit a single light particle, or photon. The arrays can be fabricated for use in optoelectronic devices, such as solar cells, which move electrons and other charge carriers.

Not all shapes were equal. The team first explored growth of the flat crystals on substrates patterned with sharp steps and trenches. Surprisingly, the growing crystals hugged these flat obstacles without changing their properties or growth rates. However, curvy surfaces required the crystals to stretch as they grew to maintain their crystal structure.



Strain-tolerant triangular monolayer crystals were grown on substrates patterned with donut-shaped pillars, as shown in scanning electron microscope (bottom) and atomic force microscope (middle) image elements. The curvature of the pillars induced strain in the overlying crystals that locally altered their optoelectronic properties, as shown in bright regions of photoluminescence (top). Image credit: Christopher Rouleau, ORNL

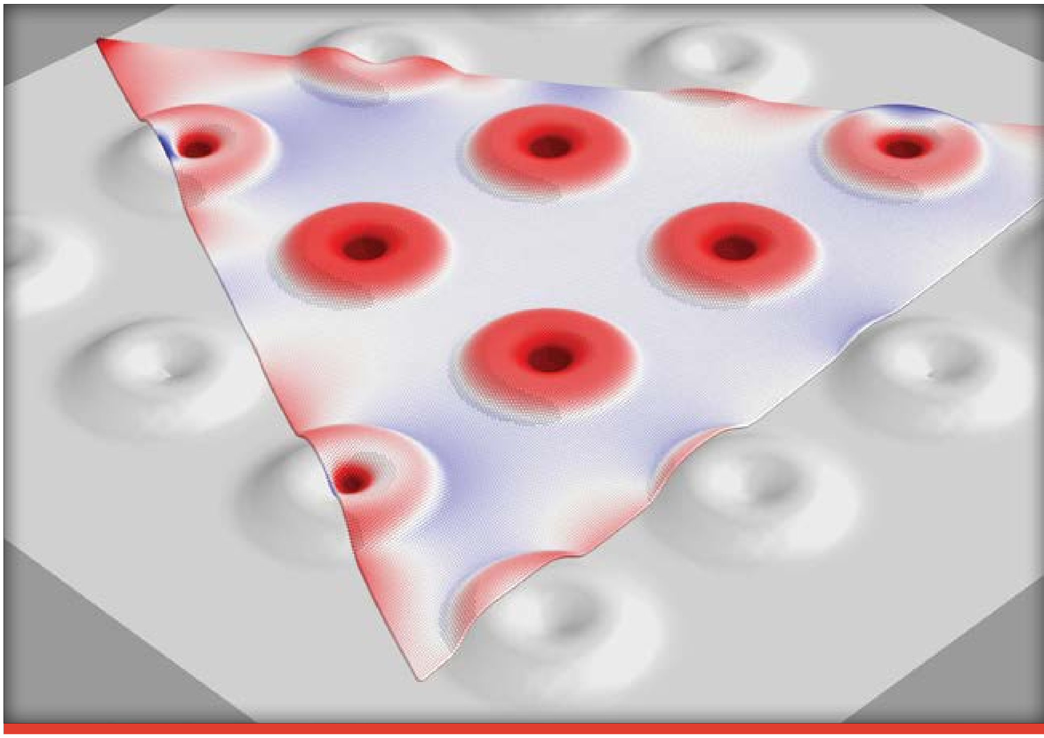
"You can engineer how much strain you impart to a crystal by designing objects for them to grow over," said Kai Xiao, who conceived the study with ORNL colleagues David Geohegan and postdoctoral researcher Kai Wang (now at Intel). "Strain is one way to make hot spots for single photon emitters."

Growing perfect 2D crystals that cling to 3D objects promises to allow strain to be placed exactly where it's needed to optimize optoelectronic properties in high-fidelity arrays of single photon emitters. Stretching or compressing the crystal lattice changes electronic structures that largely determine the behavior of electrons and holes—charge carriers—in the material. Using strain engineering, researchers can funnel these charge carriers to act precisely where desired in the crystal instead of at random defect locations.

At ORNL, Wang and Xiao designed experiments with cleanroom engineer Bernadeta Srijanto to explore the growth of 2D crystals over various nanoscale shapes in specific patterns. Srijanto first used photoresist polymer to protect certain areas of a silicon oxide surface during exposure to light and then etched away the exposed surfaces to leave vertically standing shapes, including donuts, cones and steps.

Wang and another postdoctoral researcher, Xufan Li (now at Honda Research Institute), then inserted the resulting substrates into a furnace, where vaporized tungsten oxide and sulfur reacted to deposit tungsten disulfide on the substrates as monolayer crystals. The crystals grew as an orderly lattice of atoms in perfect triangular tiles that grew larger with time by adding row after row of atoms to their outer edges. While the 2D crystals seemed to effortlessly fold like paper over tall steps and sharp trenches, growth over curved objects forced the crystals to stretch to maintain their triangular shape.

The scientists found that "donuts" 40 nanometers high were great candidates for single photon emitters because the crystals could reliably tolerate the strain they induced, and the maximum strain was precisely in the "hole" of the donut.



A theoretical simulation of the strain distribution of a triangular monolayer crystal grown on an array of donuts patterned on a substrate. Image credit: Henry Yu, Rice University.

> *"You can engineer how much strain you impart to a crystal by designing objects for them to grow over. Strain is one way to make hot spots for single photon emitters.*
>
> — Functional Hybrid Nanomaterials Group researcher **Kai Xiao**

Wang and ORNL colleague Alex Puretzky used light reflections to map the starting points for growth of crystals and the speed with which each edge of a triangular crystal progressed as it grew over the donuts. They were surprised to discover that although the crystals maintained their perfect shapes, the edges of crystals that had been strained by donuts grew faster.

To explain this acceleration, Puretzky developed a crystal growth model, and ORNL colleague Mina Yoon conducted first-principles calculations. Their work showed that strain is more likely to induce sites on the growing edge of a crystal that initiate growth, allowing it to grow faster than before.

To understand how the curvature of the donut-shaped objects dynamically localized strain in the crystal, the experimentalists consulted Boris Yakobson at Rice University—and his students Henry Yu and Nitant Gupta—to employ their phase-field modeling approach to simulate and map how curvature of the donuts induces strain during crystal growth.

The 2D crystals can be stretched to a limit by conforming to the substrate's curves. Eventually, however, the strain becomes too great and the crystals split to release the strain. After a crystal cracks, growth of the still-strained material proceeds in different directions for each new arm.

"The results present exciting opportunities to take two-dimensional materials and vertically integrate them into the third dimension for next-generation electronics," said Xiao.

New material phase may boost ultrathin electronics

by Dawn Levy
levyd@ornl.gov

A team from ORNL and Vanderbilt University has made the first experimental observation of a material phase that had been predicted but never seen.

The newly discovered phase couples with a known phase to enable unique control over material properties—an advance that paves the way to eventual manipulation of electrical conduction in 2D materials such as graphene.

The team made the discovery using a layered copper-containing crystal that is ferroelectric, meaning it has a constant electric dipole that can be reversed when an electric field is applied.

"These materials may become building blocks of ultrathin energy and electronics technologies," said ORNL materials scientist Nina Balke.

The observation shows properties that can be harnessed to provide materials with new functions. These properties depend on the locations of copper atoms in the crystal. The copper atoms can either sit within the layers of the crystal or become displaced into the gaps between layers—called "van der Waals gaps"—where they make weak ionic bonds with neighboring layers and form the new phase.

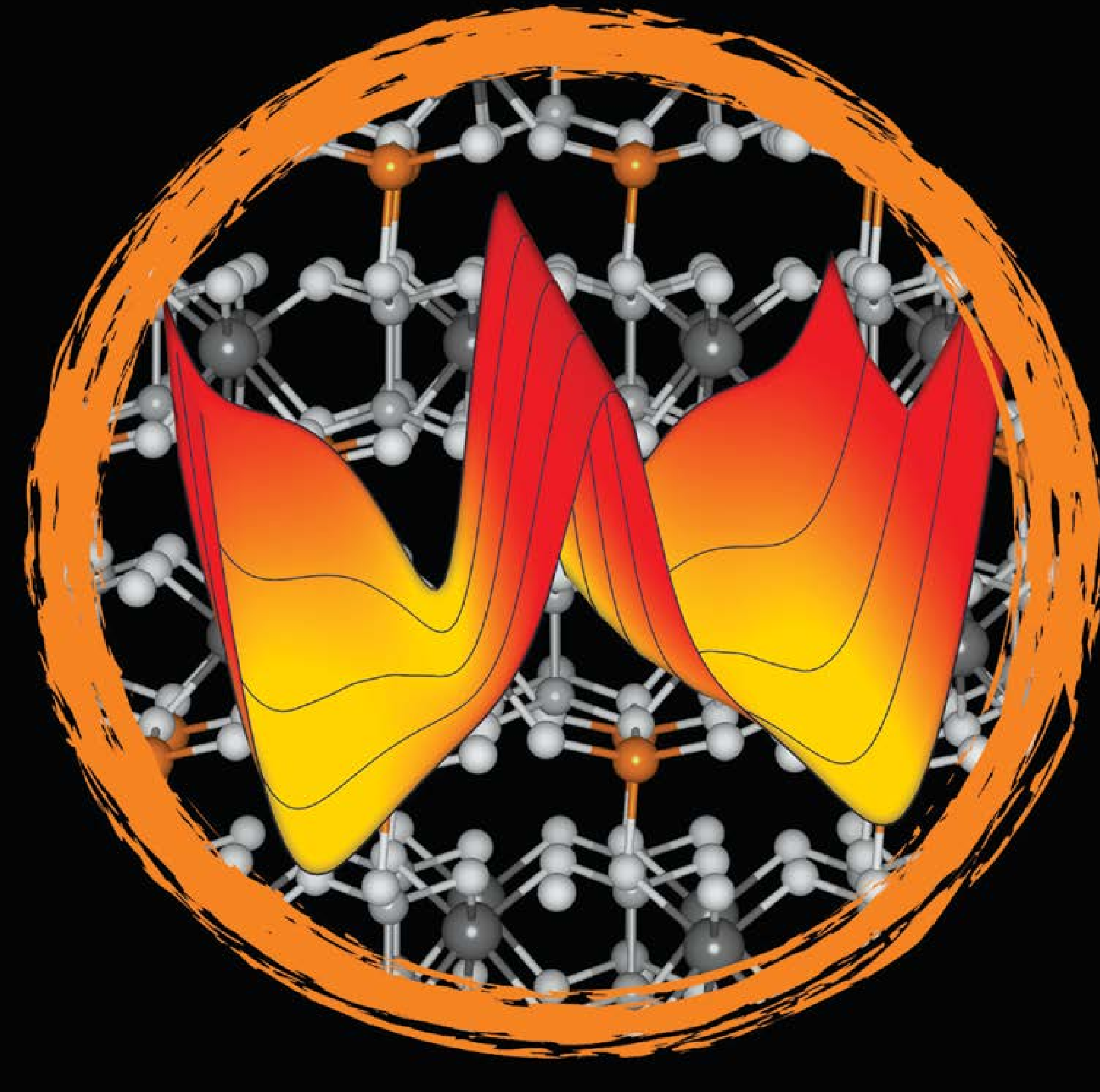
The scientists measured electromechanical responses throughout layered ferroelectric crystals of copper indium thiophosphate, or CIPS. This material is piezoelectric, meaning its surfaces become charged when it is stretched or squeezed. Conversely, applying an electric field makes a piezoelectric material expand or contract. The piezoelectric properties of CIPS were the key to studying it experimentally as well as theoretically to reveal the new phenomena.

> "This is the first reported observation of the piezoelectric and ferroelectric properties of the high-polarization phase. It was known that copper can go in the gap, but the consequences for piezoelectric and ferroelectric properties were not known.
>
> — ORNL materials scientist **Nina Balke**

The theoretical research was carried out by the research group led by Sokrates Pantelides, a professor at Vanderbilt University and distinguished visiting scientist at ORNL. Using quantum calculations, group members moved the atom responsible for polar displacement—copper—through the crystal structure and calculated the potential energy.

"A typical outcome for a ferroelectric material is that you have two energy minima, or 'wells,' for this atom; each one represents a polarization vector, one pointing up, the other down," Pantelides said. "For this material, theory predicted four energy minima, which is extremely unusual."

The research team found that the two additional energy minima arise from a second structural phase with double the polarization amplitude and with a stable position for the copper atom in the van der Waals gap. Moreover, the theoretically predicted piezoelectric constants for the two polar phases in CIPS matched the experimentally measured ones.



Van der Waals–layered CIPS has different properties depending on the locations of copper atoms (orange spheres). Unified theory and experiment led to the discovery of two coexisting phases connected through a quadruple energy well whose properties can be harnessed to provide materials with new functions. Image credit: Sabine Neumayer, ORNL

"This is the first reported observation of the piezoelectric and ferroelectric properties of the high-polarization phase," said Balke, the leading experimentalist on the team. "It was known that copper can go in the gap, but the consequences for piezoelectric and ferroelectric properties were not known. But in the end, that's what forms the quadruple well."

Sabine Neumayer, a member of the ORNL team, added, "The quadruple well opens up a lot of exciting opportunities, especially because we can control transitions between these four different polarization states using temperature, pressure and electric fields."

Usually, ferroelectrics are thought of as switches between two states. In CIPS, four states are accessible.

"CIPS is one of the first ferroelectric materials that is natively compatible with nearly all 2D materials because of its van der Waals structure," ORNL's Petro Maksymovych said. "Anytime you have van der Waals forces, it means that you can put 2D materials together and separate them without causing major structural damage. The van der Waals structure is what enables cleaving of bulk crystals to create 2D nanostructures with clean surfaces."

Scientists worldwide have been racing to create an active interface for 2D materials like graphene, a single-atom-thick material with very high electron mobility.

"We imagine that in the future, an active interface to CIPS can control graphene via piezoelectric, ferroelectric and other responsive properties," Maksymovych said. "It'll put the smarts into graphene."

New detector sees the origins of elements

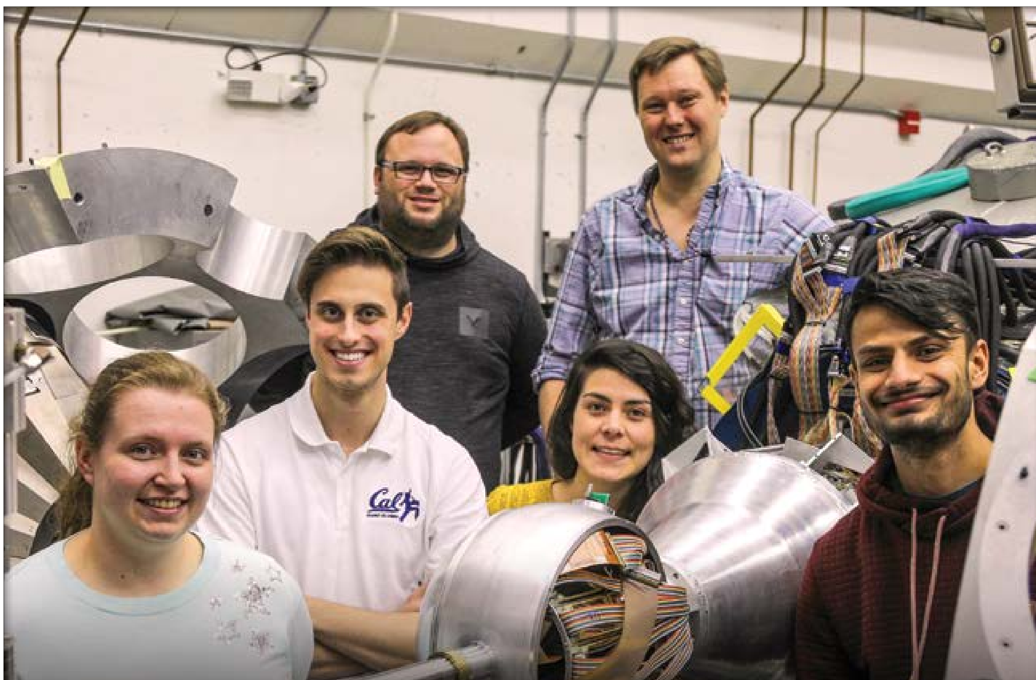
by Dawn Levy
levyd@ornl.gov

Ancient Greeks imagined that everything in the natural world came from their goddess Physis, whose name gives us the word *physics*. Present-day nuclear physicists at ORNL have created a GODDESS of their own—a detector providing insight into astrophysical nuclear reactions that produce elements heavier than hydrogen—the lightest of elements, created right after the Big Bang.

This new GODDESS grows out of a state-of-the-art charged particle detector at ORNL called the Oak Ridge Rutgers University Barrel Array. ORRUBA was created to study reactions with beams of astrophysically important radioactive nuclei. Recently, its silicon detectors were upgraded and tightly packed to prepare it to work in concert with large germanium-based gamma-ray detectors such as Argonne National Laboratory's Gammasphere and Berkeley Lab's GRETINA.

The result is GODDESS, which stands for Gammasphere/GRETINA ORRUBA: Dual Detectors for Experimental Structure Studies.

GODDESS records emissions from reactions taking place as energetic beams of radioactive nuclei gain or lose protons and neutrons and emit gamma rays or charged particles such as protons, deuterons (with one proton and one neutron), tritons (with one proton and two neutrons), helium-3 (with two protons and one neutron) and alpha particles (with two protons and two neutrons).


GODDESS is shown coupled to GRETINA with experimenters (front from left) Heather Garland, Chad Ummel and Gwen Seymour, all of Rutgers University, and Rajesh Ghimire of the University of Tennessee–Knoxville and ORNL, and (back from left) Josh Hooker of UTK and Steven Pain of ORNL.
Image credit: Andrew Ratkiewicz, ORNL

"The charged particles in the silicon detectors tell us how the nucleus was formed, and the gamma rays tell us how it decayed," explained Steven Pain of ORNL's Physics Division. "We merge the two sets of data and use them as if they were one detector for a complete picture of the reaction."

In 2019, Pain led more than 50 scientists from 12 institutions in GODDESS experiments to understand the cosmic origins of the elements.

Understanding thermonuclear runaway

One element can turn into another when protons or neutrons are captured, exchanged or expelled. When this happens in stars, it's called nucleosynthesis.

"Advanced detectors like GODDESS allow us to explore, with great sensitivity, reactions of the difficult-to-access unstable radioactive nuclei that drive the astrophysical explosions generating many of the stable elements around us," Pain said.

One experiment Pain has led focused on understanding nucleosynthesis in nova explosions—the most common stellar explosions. A nova occurs in a binary system in which a white dwarf gravitationally pulls hydrogen-rich material from a nearby companion star until thermonuclear runaway occurs and the white dwarf's surface layer explodes. The ashes of these explosions change the chemical composition of the galaxy.

University of Tennessee graduate student Rajesh Ghimire is analyzing data from that experiment, in which neutrons were transferred from deuterium in a target onto an intense beam of the short-lived radioactive isotope phosphorus-30.

The particle and gamma-ray detectors spotted what emerged, correlating times, places and energies of proton and gamma-ray production. The phosphorus-30 nucleus strongly affects the ratios of most of the heavier elements produced during a nova explosion.

Illuminating heavy-element creation

Another experiment that Pain led transmuted a much heavier isotope, tellurium-134.

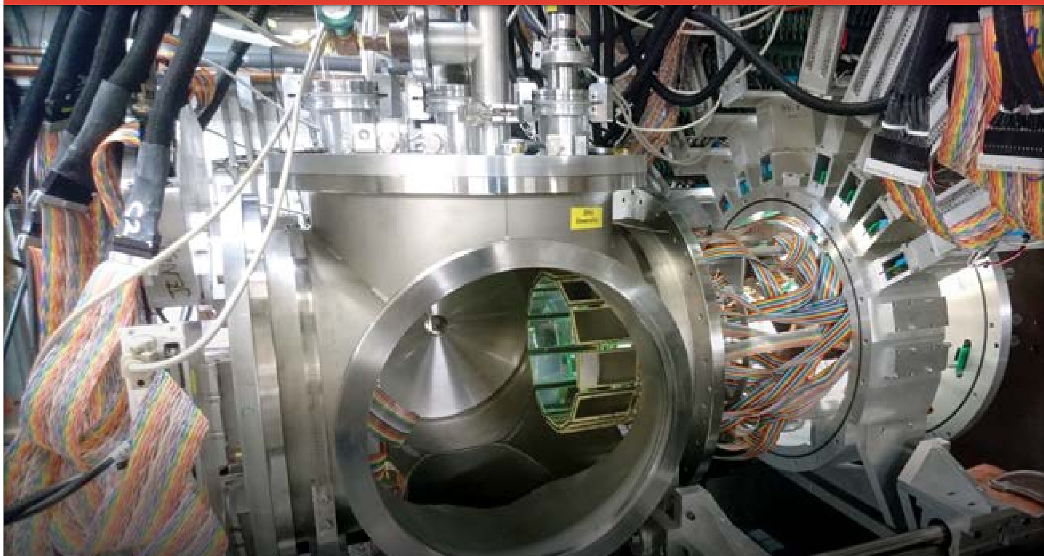
"This nucleus is involved in the rapid neutron capture process, or r-process, which is the way that half the elements heavier than iron are formed in the universe," he said. It occurs in an environment with many free neutrons, perhaps supernovae or neutron star mergers.

Understanding r-process nucleosynthesis will be a major activity at DOE's Facility for Rare Isotope Beams, or FRIB, scheduled to open at Michigan State University in 2022. FRIB will enable discoveries related to rare isotopes, nuclear astrophysics and fundamental interactions, as well as applications in medicine, homeland security and industry.

The tellurium-134 experiment made use of radioactive californium produced at ORNL and installed at the Argonne Tandem Linear Accelerator System. The californium fissions spontaneously, with tellurium-134 among the products.

Said Pain, "We're trying to understand the role of this tellurium-134 nucleus in the r-process in different potential astrophysical sites. The reaction flow in this network of neutron capture reactions affects the abundances of the elements created. We need to understand this network to understand the origin of the heavy elements."

GODDESS measures transfer reactions occurring after a radioactive beam bombards a deuterium-containing target inside a barrel of silicon detectors. "It's pretty much silicon in every direction," Pain said. "No matter where the particle comes out, we detect it." Image credit: Steven Pain, ORNL



GODDESS's ORRUBA component, shown in an early form that was not compact enough for coupling with gamma-ray detectors, will travel to Michigan State University for a stand-alone study of potassium-38 (of interest for novae studies) and for later coupling with GRETINA to explore germanium-80 (relevant to understanding the r-process). Image credit: Steven Pain, ORNL

ORRUBA now fits tidily into this 14-inch-diameter sphere. At left, a beamline directs energetic radioactive nuclei into the sphere to strike a central target. The shiny silicon detectors inside the sphere form the staves of ORRUBA's barrel. Image credit: Steven Pain, ORNL

Fake fish

test real impacts of hydropower

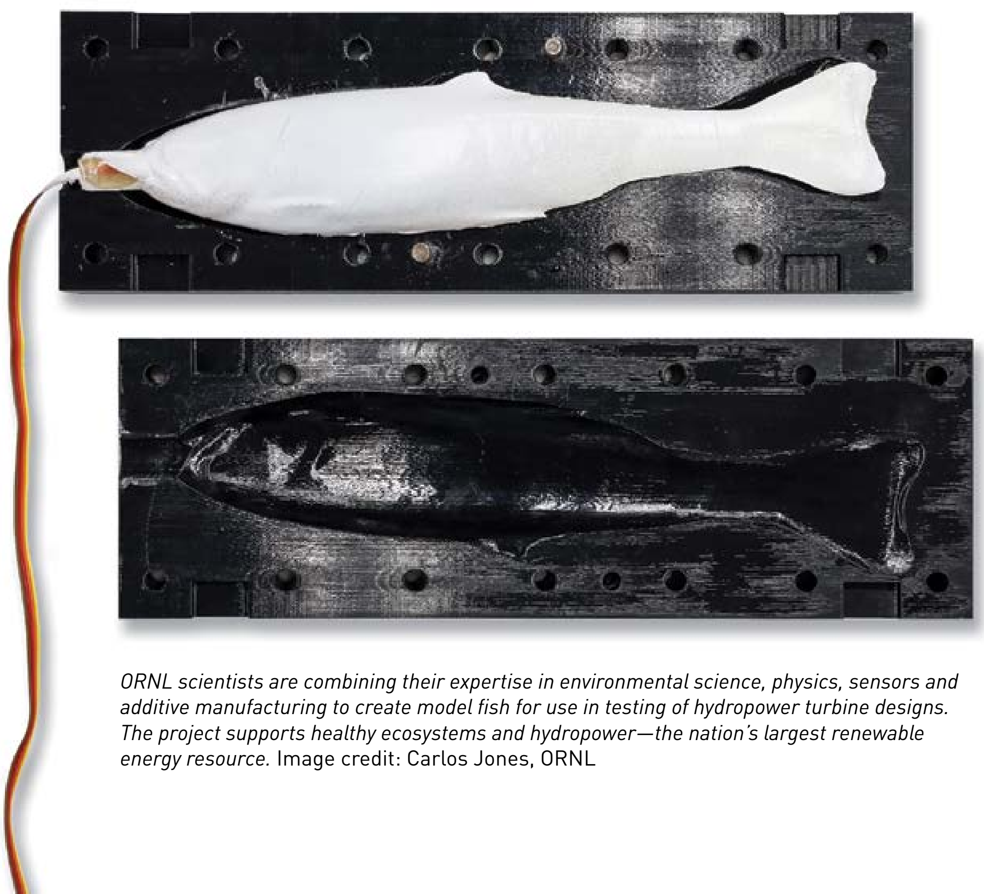
by Stephanie Seay
seaysg@ornl.gov

In the pursuit of fish-friendly hydropower, ORNL scientists landed a unique solution: using 3D printing and sensors to create fake fish for turbine testing.

As fish pass through hydropower dams, they can encounter obstacles that cause injuries—pressure changes, turbulence and spinning blades on turbines. There are many factors to take into account when testing hydropower impacts on fish: how fast the blades are moving, the thickness and angle of the blades, how big each fish is and where its center of mass sits. By creating model fish, ORNL researchers can analyze the impact of turbine designs as part of their environmental assessment work for hydropower projects without using live subjects.

"We want to understand the forces different fish species encounter and how those forces may result in injury or mortality," said Ryan Saylor, a Bredesen Center for Interdisciplinary Research and Graduate Education student working in ORNL's Environmental Sciences Division. "There may be tweaks that turbine designers and manufacturers could make that would conserve fish species while at the same time minimizing the impact on energy production."

The work is important; hydropower accounts for 6 percent of the country's elec-



ORNL scientists are combining their expertise in environmental science, physics, sensors and additive manufacturing to create model fish for use in testing of hydropower turbine designs. The project supports healthy ecosystems and hydropower—the nation's largest renewable energy resource. Image credit: Carlos Jones, ORNL

tricity generation. ORNL has a long history of supporting these projects, including improvements to the licensing and regulatory process.

The scientists decided to create a model fish—in technical terms, a biomimetic test device—to help them understand the forces of the turbine blades and generate multiple data points for analysis. They came up with the idea of using ballistic gel for the fish body. The gel, originally developed for military purposes, can be modified with different densities to mimic muscle tissue.

To create molds for various fish species, the researchers turned to the 3D-printing capabilities at the Manufacturing Demonstration Facility, a DOE designated user facility at ORNL. The researchers brought fish to the MDF to be laser-scanned, and the resulting contours were fed into a computer-aided design program that in turn guided a 3D printer to create molds of each fish to be tested.

Brian Post, who led the MDF effort, noted that 3D printing the molds is a fast, low-cost solution that allows for the creation of a large variety of fish models in a short period of time.

"Each species has a different morphology, so making molds allows us to capture those differences. We can make a one-of-a-kind fish pretty easily. If you were to conventionally produce the molds, it would take longer to subtract the shape out of a block of material," Post said.

The environmental scientists mixed the ballistic gel with cinnamon oil (an inexpensive antimicrobial agent), filled the molds and allowed the gel to set. The team tested the "squishiness" of subsequent fake fish to get as close as possible to reality. The scientists then coated the fish in a plastic-like paint to give them more rigidity and to mimic skin and scales.

Sensors embedded in the models measure acceleration and g-forces in the turbine simulator in three dimensions. Strain gauges are also used to measure how the fish stretch or contract internally and externally as a result of the simulated strikes.

"Each species has a different morphology, so making molds allows us to capture those differences. We can make a one-of-a-kind fish pretty easily. If you were to conventionally produce the molds, it would take longer to subtract the shape out of a block of material.

— **Brian Post** of the Manufacturing Science Division

The scientists continue to improve their models, including increasing the sampling rates, which in turn should result in higher-resolution data and enable advances in data extraction and analysis. So far they have created and tested models of five fish species: rainbow trout, bluegill, shad, bass and eel.

"Mimicking biology is difficult," Saylor noted. "We've worked to get as close as we can to a good representation without the use of specialized equipment that could increase costs."

New tool

offers a better picture of plants

by Kim Askey
askeyka@ornl.gov

Scientists have a powerful new tool in the quest to produce better plants for biofuels, bioproducts, agriculture and more.

A system of sophisticated robotics and sensors in ORNL's new Advanced Plant Phenotyping Laboratory, or APPL, collects an unprecedented amount of data on plant characteristics called phenotypes.

The automated system propels 500 large plants along more than 700 feet of track, sending them on a winding path through the imaging stations. During a typical experiment, the system collects terabytes of data, presenting both a challenge and tremendous opportunities for discovery.

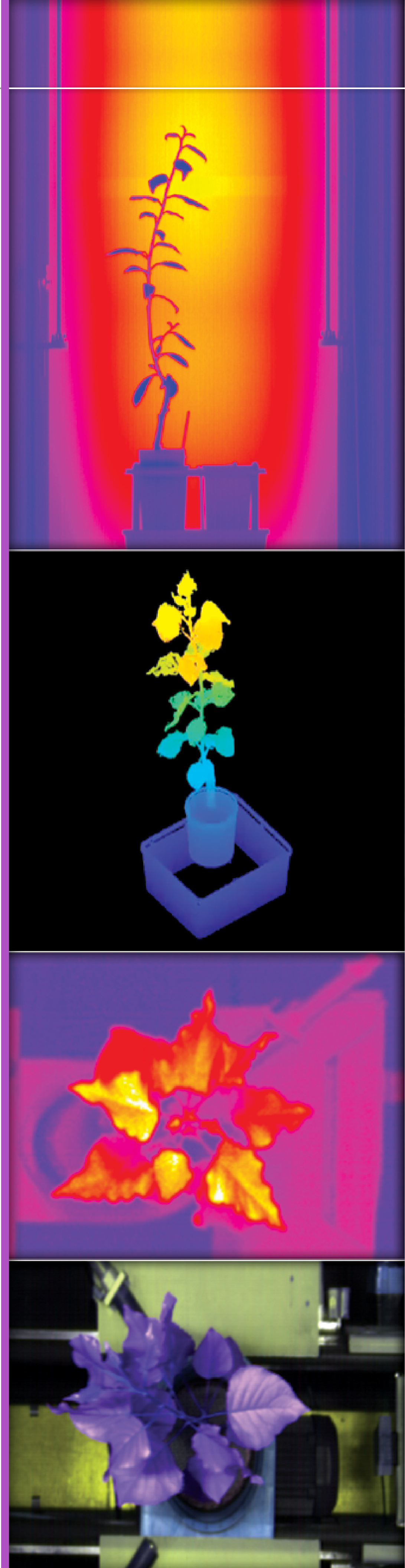
Among its many capabilities, APPL allows scientists to investigate sustainability traits such as drought resistance in poplar and switchgrass and to examine how those traits translate across scales, from the molecular to the cellular to the whole plant and, ultimately, to the ecosystem. These new capabilities will also enable researchers to identify the impacts of microbes on plant growth and productivity.

APPL offers the world's most diverse suite of imaging capabilities. An array of five imaging stations provides RGB (red–green–blue), hyperspectral, thermal, fluorescence and 3D laser imaging that captures plant growth, photosynthetic activity, changes in water and nitrogen distribution and much more.

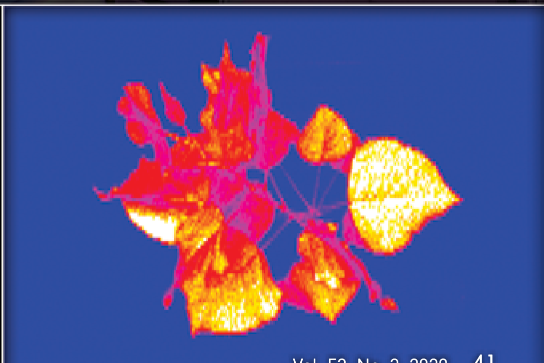
"We're fortunate that we're located here at ORNL," said Jerry Tuskan, director of the DOE Center for Bioenergy Innovation. "We've got experts developing machine learning algorithms and using the laboratory's supercomputing resources to combine these data into a 3D visualization of each plant that reveals its structural and chemical properties in high-resolution detail."

To achieve this detailed 3D visualization, the phenotyping system must capture images with the extreme precision that only automation can provide. Scientists hope to see cues and signals in these visualizations that indicate shifts in plants' activity due to conditions like drought stress or pathogen attacks.

"This potential to predict changes before they are visually apparent is exciting," continued Tuskan. "This is unexplored territory."



The Advanced Plant Phenotyping Laboratory (large image) uses an array of imaging capabilities, including (from top left to bottom right) thermal, 3D laser scan, hyperspectral short wavelength infrared, hyperspectral visible to near infrared, RGB (red-green-blue), binary plant mask, and fluorescence imaging.
Image credits (photograph): Genevieve Martin, ORNL. Image credits (phenotype imaging): ORNL



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.

Allen Scheie

Postdoc, Neutron Scattering Division
Ph.D., Condensed Matter Physics, Johns Hopkins University
Hometown: Cincinnati, Ohio

What are you working on at ORNL?

I am searching for new magnetic quasiparticles using neutron scattering. Quasiparticles like the electron hole are the foundation for modern electronics, and a long list of them has been theoretically predicted but not experimentally identified. My research seeks to identify these predicted quasiparticles in magnetic materials using neutron scattering.

What would you like to do in your career?

I would like to contribute to discoveries that change how we think about nature, especially concerning emergent properties of complex systems. I am also passionate about communicating science, and I hope to be able to explain both my results and the scientific process in a way that nonexperts can understand.

Why did you choose a career in science?

I chose a career in science because I was fascinated by nature following precise, mathematical laws. The fact that creation is so well-ordered and comprehensible fascinated me, and it continues to fascinate me.

Tugba Turnaoglu

Postdoc, Buildings and Transportation Science Division
Ph.D., Chemical and Petroleum Engineering, University of Kansas
Hometown: Ankara, Turkey

What are you working on at ORNL?

The foundation of our research group is to carry the fundamentals of science and engineering to the most innovative, sustainable, and energy-efficient building equipment technologies. My work is focused on improving and developing the technologies for a wide range of equipment, from dishwashers to advanced dehumidification units.

What would you like to do in your career?

I would like to build my team to carry on fundamental and applied research to combat the challenges of the 21st century on the pillars of advanced materials and the innovative design of processes and systems.

Why did you choose a career in science?

At an early age, I discovered I enjoy scientific discussions. My endless passion for learning new things and my scientific curiosity led me to be a scientist. Also, I have always been inspired by the lives of famous scientists and the paths they followed in pursuit of remarkable discoveries.

Obed D. Acevedo Román

Graduate student, Materials Science and Technology Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Vega Baja, Puerto Rico

What are you working on at ORNL?

My research is focused on the metallurgy of steel components made via large-scale additive manufacturing and nickel-based superalloys. My mission is to understand the phenomena that occur during deposition to provide insight that will help optimize these processes.

What would you like to do in your career?

Additive manufacturing is a field that is expanding very rapidly, and I would like to contribute to this growth by helping solve the challenges that come with it. We can reduce a lot of time and material waste by adapting these technologies to many different applications.

Why did you choose a career in science?

I have always been fascinated by metals, and the research I work on provides new challenges every day, which makes for a rather exciting career. I take pride in knowing that the work we do has a positive impact and promotes cleaner energy.

Sujana Chandrasekar

Graduate student, Electrification and Energy Infrastructures Division
Ph.D. student, Data Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Chennai, India

What are you working on at ORNL?

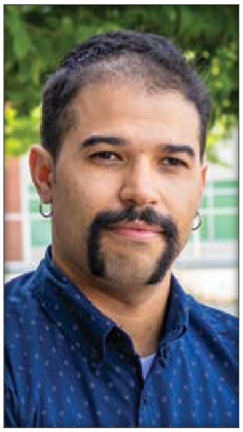
I work on developing data science tools to understand additive manufacturing processes. Additive manufacturing, or 3D printing, results in variation in material properties, leading to challenges in qualifying parts for use. My research is on time series methods for monitoring thermal process conditions in AM, potentially paving the way for data-driven part qualification.

What would you like to do in your career?

I would like to pursue research on data science, particularly for manufacturing and industrial processes, where there is immense potential for data-driven decision-making. On this journey, I want to continue learning, exploring and developing novel algorithms and applications. I enjoy teaching as a two-way learning process and would like to mentor students.

Why did you choose a career in science?

I enjoyed math and science in middle and high school, where I was immensely fortunate to have fantastic teachers. With my parents having strong math and physics backgrounds, I saw science as a natural career option. For me, the pull of data science lies in seeing the beauty of math shine through in diverse applications.



Daniel Claudino

Postdoc, Computer Science and Mathematics Division
Ph.D., Chemical Physics, University of Florida
Hometown: São Paulo, Brazil

What are you working on at ORNL?

I work where quantum chemistry meets quantum computing and software engineering. I develop software for theoretical simulations of chemistry at the molecular level by leveraging the integration of supercomputers such as ORNL's Summit and quantum processors, which have the prospect of greatly surpassing the current computer technologies.

What would you like to do in your career?

I aim to be at the forefront of software development for domain applications of quantum computers, exploiting the synergy between different computing paradigms, broadening the scope of these applications to other problems in the physical sciences and allowing impactful contributions in key areas such as discovery of new drugs and materials.

Why did you choose a career in science?

I have always found it fascinating that even quite complex natural phenomena lend themselves to mathematical models. A career in science was a no-brainer when I became aware that computers could be powerful tools in bringing many of these models to life, furthering our understanding of nature as a whole.

Samantha Peters

Graduate student, Chemical Sciences Division
Ph.D. student, Genome Science and Technology, University of Tennessee
Hometown: Lakewood, Colorado

What are you working on at ORNL?

My research involves integrating mass spectrometry–based metaproteomics to study the functionality of the human gut microbiome pertaining to community establishment and degradation of dietary fibers. This work will help us understand the functional roles of microbes as drivers of human health and disease.

What would you like to do in your career?

I want to pursue mass spectrometry advancements that drive biological research. Along with research aimed at technological advances, I am very interested in continuing to explore microbial dynamics—specifically related to community-level function, competition, and cooperation among constituent microbes and host–microbe interactions as they pertain to host health and disease.

Why did you choose a career in science?

I love that science is an unfinished story; there are so many unanswered questions that must be addressed for a better understanding of the natural environment. Answering these questions will help in finding solutions to incredibly complex problems.

The origins of fusion energy research at ORNL

E.D. Shipley led ORNL's earliest explorations of controlled fusion energy starting in the early 1950s. Image credit: ORNL

by Bonnie Nestor
nestormb@ornl.gov

ORNL is building on a long legacy of leadership in fusion energy—the process that powers stars—by managing the U.S. contributions to the international ITER project, designing the Material Plasma Exposure Experiment and working in a variety of other ways to enable the deployment of practical fusion energy systems.

An official history published by the Atomic Energy Commission in 1958 says that ORNL became involved when "a small group with extensive experience in ion-source technology became interested in participating in the controlled fusion field. Under the direction of E.D. Shipley, theoretical studies were initiated in the latter part of 1952 and later supplemented by an experimental investigation of several topics of general interest to the Sherwood effort."

Project Sherwood was the AEC's code name for a classified program that was launched soon after the president of Argentina announced in March 1951 that researchers in that country had demonstrated controlled nuclear fusion. The results from Argentina were quickly found to be spurious, but the AEC proceeded to fund experiments at Los Alamos and Livermore laboratories and at Princeton University while supporting smaller efforts at ORNL and New York University.

Shipley, who had co-founded the electrical engineering department at the University of Tennessee, Knoxville, joined the Manhattan Project in Oak Ridge in 1944. He was director of research and development at the Y-12 Plant when three Y-12 divisions were transferred to ORNL in 1950. Shipley also transferred to ORNL, becoming an assistant research director with oversight for the new ORNL divisions.

One of these, the Electromagnetic Research Division, had its roots in a group of University of California researchers who came to Y-12 in 1943 to work on the calutrons used for electromagnetic separation of uranium. After electromagnetic separation at Y-12 was shut down, division staff took advantage of the calutrons and their infrastructure to explore new opportunities in isotope production and nuclear physics research.

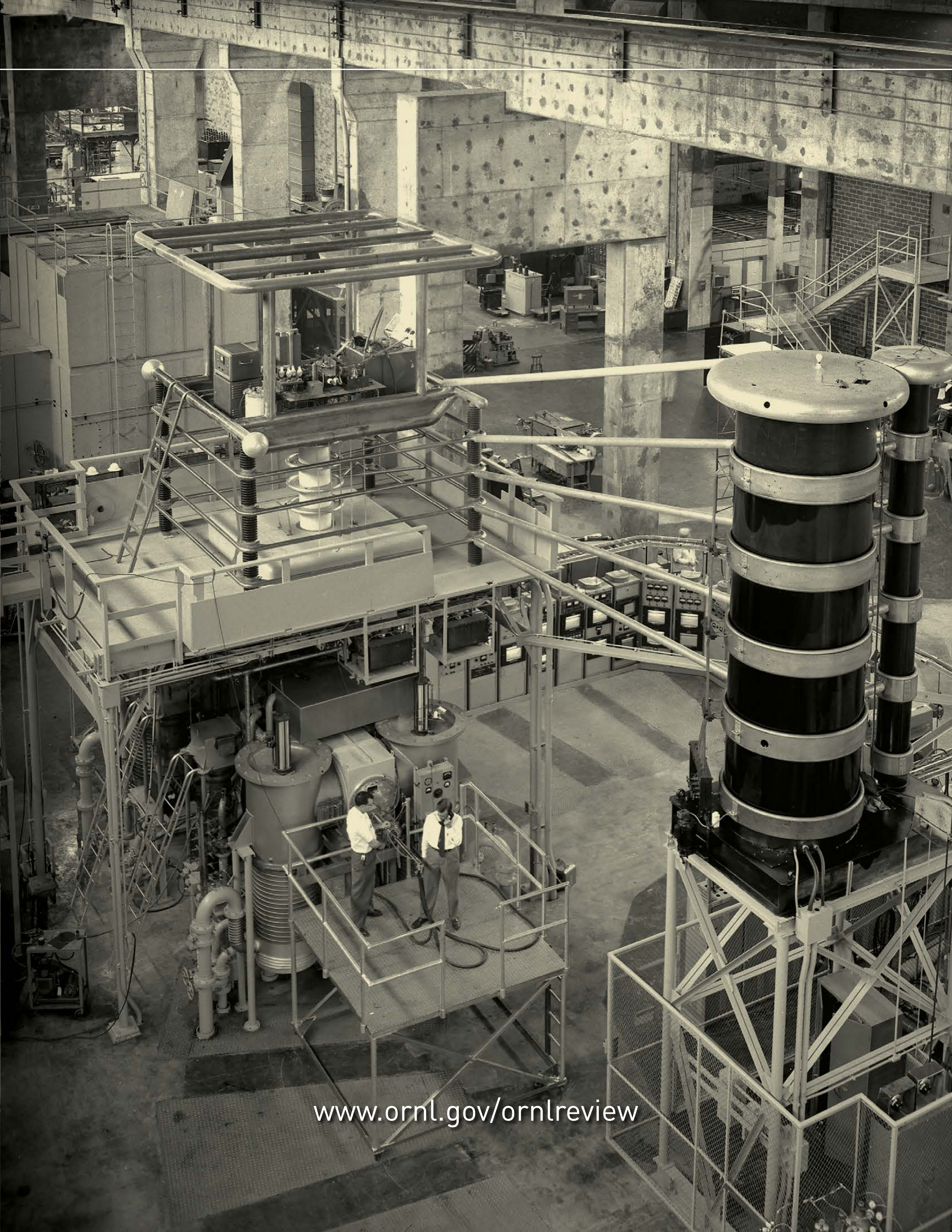
One staff member, John S. Luce, would eventually receive more than a dozen patents for inventions related to ion sources and their application to fusion research. Luce also led the development of ORNL's first large-scale fusion device, the Direct Current Experiment, or DCX, which began operating in 1957.

ORNL's early theoretical studies were led by Albert Simon, who was first a Physics Division staff member and then associate director of the Applied Nuclear Physics Division. Late in 1955, he presented a series of nine "Project Sherwood orientation lectures" to staff at Oak Ridge.

Access was tightly controlled; Project Sherwood remained classified until 1957, the same year that ORNL's Thermonuclear Experimental Division was created with Shipley as its first director. With the development of two operating models of DCX, which were exhibited in Geneva in September 1958 at the Second United Nations International Conference on the Peaceful Uses of Atomic Energy, Oak Ridge moved into the forefront of the international fusion community.

Simon's first Project Sherwood lecture predicted an increasing global demand for energy and the potential of fusion to solve the world's energy problems "for an essentially infinite time." Although early optimism about fusion power faded as researchers gained a better understanding of its complex physics and engineering challenges, the promise of clean, abundant energy remains the driver for fusion R&D around the world.

The Direct Current Experiment, ORNL's first large-scale fusion device, began operating in 1957. Image credit: ORNL



www.ornl.gov/ornlreview

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

PRSRT STD
US Postage
PAID
Permit No. 3
Oak Ridge, TN

Editor—Leo Williams
Writers—Kim Askey, Paul Boisvert, Abby Bower, Kristi Nelson Bumpus, Karen Dunlap, Adriana Ghiozzi, Rachel Harken, Scott Jones, Dawn Levy, Bonnie Nestor, Jim Pearce, Elizabeth Rosenthal, Stephanie Seay, Sara Shoemaker, Leo Williams
Designer—Brett Hopwood
Illustrators—Nathan Armistead, Jill Hemman, Michelle Lehman, Adam Malin
Copy editor—Laurie Varma
Photographers—Carlos Jones, Genevieve Martin, Jason Richards
Stock images—**getty**images™

Phone: (+1) 865.574.8891
Fax: (+1) 865.574.0595
E-mail: ornlreview@ornl.gov
Internet: www.ornl.gov/ornlreview

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

ISSN 0048-1262