OAK RIDGE NATIONAL LABORATORY

Review

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Oak Ridge National Laboratory

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OAK RIDGE NATIONAL LABORATORY
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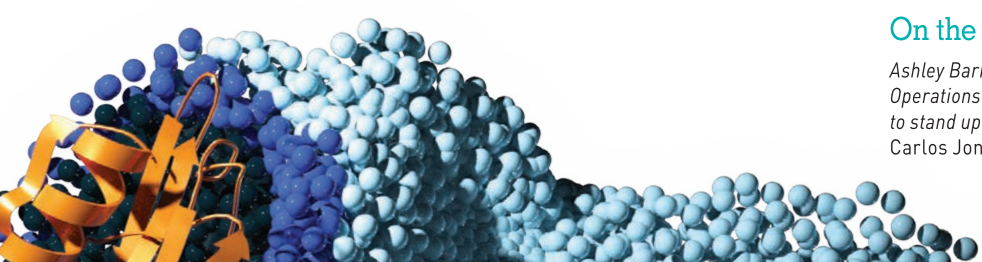


On the Cover

Ashley Barker, who leads the Oak Ridge Leadership Computing Facility's Operations Section, is among the many ORNL staff who worked day and night to stand up the world's first exascale supercomputer, Frontier. Image credit: Carlos Jones, ORNL

Making an exascale impact with Frontier

Oak Ridge National Laboratory is proud to be home to the world's most powerful supercomputer, but Frontier's almost incomprehensible speed shouldn't distract from the most important question:

So what?

Why does it matter that Frontier can perform a quintillion calculations per second? Or that it contains 60 million components and 90 miles of interconnect cables? Or that it covers the equivalent of two basketball courts and requires 30 megawatts of power?

It's undoubtedly a noteworthy feat of engineering, but what matters most is the scientific discovery that Frontier enables:

- General Electric has already used Frontier to develop models for new airplane engines that could reduce carbon dioxide emissions more than 20 percent.
- Medical researchers will leverage Frontier's artificial intelligence and machine learning power to deepen their understanding of cancer and other diseases, and to discover new drugs to fight them.
- Scientists are working to model earthquakes at levels of detail impossible without Frontier's power, simulating how waves traveling through the earth affect building structures.

In this issue of *ORNL Review*, we pull back the curtain on Frontier's first year (see "Exascale impact: The Frontier supercomputer gets to work," page 8), including the herculean effort that went into making the system a reality (see "ORNL's methodical leap into the exascale era," page 14) and its specific application to pioneering nuclear energy (see "Exascale tools for developing new reactors," page 16).

As we show, much credit goes to the staff of the Oak Ridge Leadership Computing Facility and its industry partners from Hewlett Packard Enterprise and AMD. Their jobs are definitely not over (see "OLCF teams fine-tune Frontier for science," page 18), but we know they'll continue to make Frontier one of the most productive scientific tools ever seen.

Also in this issue of *ORNL Review*, you'll learn how researchers:

- Create the first identified nanoscale structure in which memory can be encoded (See "Cell membrane discovery heralds computing advances," page 24).
- Make natural gas furnaces cleaner by developing an add-on technology that removes more than 99.9 percent of acidic gases (see "Add-on device makes home furnaces cleaner," page 30).
- Design a microorganism for converting mixed plastic into sustainable products (see "Tiny, revved-up microbe tackles big plastics challenge," page 36).
- Explore the potential of hydrogen as a railway fuel (see "Researchers explore hydrogen power for railways," page 44).

We look back at the career of former ORNL physicist and University of Tennessee professor Katharine Way, a data pioneer committed to understanding nuclear reactions and decay products (see "Kay Way: The mother of nuclear data," page 50).

Today, ORNL is committed to working with stakeholders across East Tennessee to develop a workforce for the nuclear industry of tomorrow (see "East Tennessee looks to bolster nuclear workforce," page 40).

Finally, in Research Insights, our technical staff shine a light on additive manufacturing, including its application in carbon capture, radiation detection and nuclear fuel (see "Additive Manufacturing the Future, Part I: Applications for Additive Manufacturing," page 52).

I'm sure you'll see this *Review* is another testament to what can be accomplished when good people from diverse fields work together.

Jeff W. Smith
Interim Laboratory Director

Stephen Streiffer

Stephen Streiffer named next director of ORNL

UT-Battelle, LLC, has appointed Stephen K. Streiffer to be the next director of ORNL. He most recently served as interim director at SLAC National Accelerator Laboratory and will join ORNL on Oct. 16.

"Stephen is a proven leader with diverse experience and a commitment to mission-driven research and development," said Lou Von Thaer, CEO of Battelle and chair of UT-Battelle, which operates ORNL for the Department of Energy. "Throughout his career, Stephen has leveraged existing strengths to create new opportunities and partnerships that strengthen our nation's ability to innovate and compete."

Streiffer joined SLAC last year as Stanford University's vice president responsible for oversight of the lab. He was named interim director in February 2023. He previously spent 24 years in research and leadership positions at Argonne National Laboratory, concluding his tenure as the lab's deputy director for science and technology.

"Our national laboratories provide scientists with access to some of the most powerful research facilities in the world, and Stephen has been a key leader in the development of these capabilities," said Asmeret Asefaw Berhe, director of DOE's Office of Science. "At Oak Ridge, Stephen's experience will help to ensure continued impact that benefits the nation and world."

At Argonne, Streiffer led the Photon Sciences Directorate and served as director of the Advanced Photon Source, a DOE Office of Science user facility that generates ultra-bright, high-energy X-ray beams for researchers from government, academia and the private sector. APS is undergoing an $815 million upgrade.

Streiffer earned his Ph.D. in materials science and engineering from Stanford University and a bachelor's in materials science from Rice University. He is a fellow of the American Physical Society and a member of the Materials Research Society and Institute of Electrical and Electronics Engineers.

"I look forward to getting to work at Oak Ridge," Streiffer said. "Through my roles with Office of Science programs and user facilities, I've collaborated with ORNL and its extremely talented staff for many years. It's a great honor to be selected as lab director and to join the team, and I'm committed to continuing the transformative role Oak Ridge has played in our nation's scientific enterprise for almost 80 years." — *Leo Williams*

Recyclable composites help drive net-zero goal

ORNL scientists have designed a recyclable polymer for carbon-fiber composites to enable circular manufacturing of parts that boost energy efficiency in automotive, wind power and aerospace applications.

Carbon-fiber composites, or fiber-reinforced polymers, are strong, lightweight materials that can help lower fuel consumption and reduce emissions in critical areas such as transportation. However, unlike metal competitors, carbon-fiber composites are not typically recyclable, meaning wider adoption could present waste challenges.

"Our goal is to extend the lifecycle of these materials by making reuse possible without sacrificing performance," said ORNL's Md Anisur Rahman.

The team's approach incorporates dynamic covalent bonds that are reversible, enabling both carbon-fiber and polymer recycling. The new polymer maintained mechanical strength in six reprocessing cycles, a sharp contrast to previously reported polymers.

"ORNL's carbon-fiber composites enable fast processing and can be repaired or reprocessed multiple times, opening pathways to circular, low-carbon manufacturing," said ORNL's Tomonori Saito. — *Ashley Huff*

ORNL researchers designed a recyclable carbon fiber material to promote low-carbon manufacturing. Image credit: Chad Malone, ORNL

A better technique for battery manufacturing

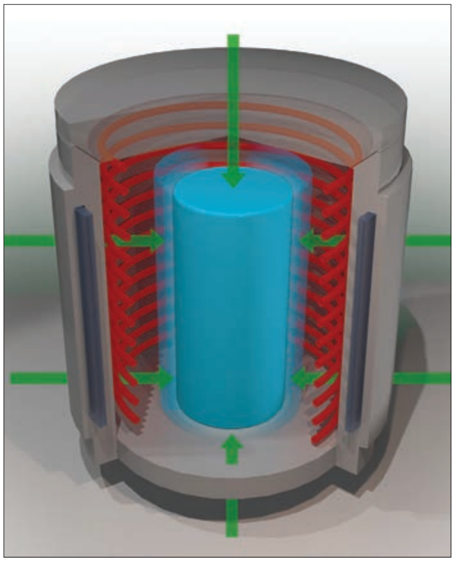
Following months of promising test results, ORNL battery researchers are recommending that the solid-state battery industry focus on a technique known as isostatic pressing as it looks to commercialize next-generation batteries.

Commercial-scale production of solid-state batteries is a goal for electric vehicle manufacturers because these batteries have the potential to charge faster, last longer and operate more safely than the lithium-ion batteries currently on the market.

In a focus review paper for *ACS Energy Letters*, ORNL researchers recommend attention be given to the little-studied isostatic pressing approach. This process uses fluids and gases like water, oil or argon inside a machine to apply consistent pressure across a battery component, creating a highly uniform material. With the help of an industry partner that produces this pressing equipment, ORNL researchers found that isostatic pressing could make battery production easier and faster while creating better conditions for energy flow.

When a battery charges or discharges, ions move through an electrolyte between its positive and negative poles, which are made of thin layers of metal. In the lithium-ion batteries that power everything from cell phones to electric vehicles, the electrolyte is a liquid through which ions travel easily. Unfortunately, this liquid can also spill or ignite if the separation between battery layers is compromised.

ORNL's Marm Dixit and colleagues found that isostatic pressing can create thin layers of solid, uniform electrolyte, maintaining a high level of contact between the layers for smooth ion movement. The method works with a variety of battery compositions at different temperatures and pressures.



Isostatic pressing applies consistent heat and pressure from all directions across a battery component within a chamber. Image credit: Andy Sproles

Among the promising results, isostatic pressing was found to be extremely successful at low temperatures and with soft electrolyte materials, which are easier to process and which have favorable crystal structures for ion movement. Previously, isostatic pressing of batteries had been done mostly at extremes: very high temperatures or room temperature, but not in between. — *S. Heather Duncan*

For more information: http://bit.ly/43d8NTV

Sutharshan named deputy for operations at ORNL

Balendra Sutharshan has been named chief operating officer for ORNL, serving as ORNL's deputy for operations and as executive vice president, operations, for UT-Battelle LLC. He succeeds Alan Icenhour, who retired this spring after serving in the role since 2021. UT-Battelle operates ORNL for the Department of Energy.

Sutharshan joined ORNL in February 2021 as the associate laboratory director for the Isotope Science and Engineering Directorate. Under his leadership, ISED achieved remarkable growth in isotope research and development, as well as production to meet the increased demand for isotopes used in medicine, research and security.

"Balendra brings comprehensive experience to the position, including an extensive knowledge of ORNL's nuclear capabilities, strong relationships across the national lab and Battelle systems, and a history of driving operational performance improvements and organizational strategy," interim ORNL Director Jeff Smith said. "I am excited for Balendra to serve in this important role for ORNL."

During Sutharshan's tenure as ALD, ISED deployed new enrichment technology capabilities and stewarded new projects that will help to secure the domestic isotope supply chain, including the Stable Isotope Production and Research Center, the Stable Isotope Production Facility and the Radioisotope Processing Facility. He established the Isotope Processing and Manufacturing Division in 2022 to further improve production performance and introduced predictive maintenance into the lab's hot cell facilities to reduce downtime.

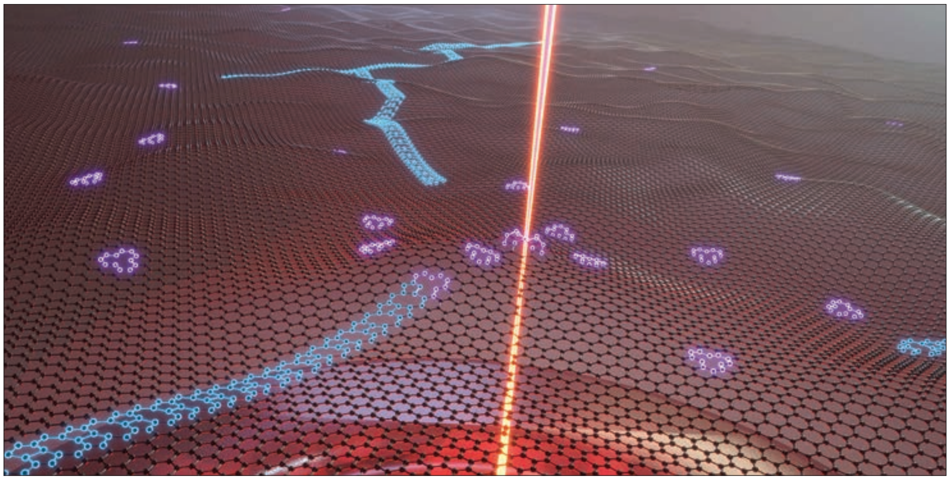
Balendra Sutharshan

"It's an honor to be part of an organization that empowers leaders and teams to pursue breakthrough science and technology and has roots back to the Manhattan Project," Sutharshan said. "I look forward to strengthening ORNL's operations and facilities strategies and continuing to support the lab's engagement with communities where we work and live." — *Sara Shoemaker*

New insights advance atomic-scale manufacturing

ORNL researchers serendipitously discovered when they automated the beam of an electron microscope to precisely drill holes in the atomically thin lattice of graphene, the drilled holes closed up. They expected the heat to make atoms easier to remove, but they saw the opposite effect.

"Graphene appeared impervious to the electron beam," said Ondrej Dyck, who co-led the study with Stephen Jesse at ORNL's Center for Nanophase Materials Sciences. Jesse added, "It heals locally,



When an electron beam drills holes in heated graphene, single-atom vacancies, shown in purple, diffuse until they join with other vacancies to form stationary structures and chains, shown in blue.
Image credit: Ondrej Dyck, ORNL

like the (fictitious) liquid-metal T-1000 in the movie Terminator 2: Judgment Day."

Theory-based computations performed on the lab's Summit supercomputer, led by ORNL's Mina Yoon, explained the quasi-metal's healing ability: Single atomic vacancies zip through the heated graphene until they meet up with other vacancies and become immobilized.

"Similar processes are likely to extend to other 2D materials," Dyck said.

"Controlling such processes could help us realize graphene's promise for quantum information science," Jesse said.

The researchers are applying this new knowledge to guide creation of atomic-scale devices. — *Dawn Levy*

New molecule disrupts SARS-CoV-2 infection

An ORNL-led team has designed a molecule that disrupts the infection mechanism of the SARS-CoV-2 coronavirus and could be used to develop new treatments for COVID-19 and other viral diseases.

The molecule targets a lesser-studied enzyme in COVID-19 research, PLpro, that helps the coronavirus multiply and hampers the host body's immune response. The molecule, called a covalent inhibitor, is effective as an antiviral treatment because it forms a strong chemical bond with its intended protein target.

"We're attacking the virus from a different front, which is a good strategy in infectious disease research," said Jerry Parks, who led the project and leads the Molecular Biophysics group at ORNL.

The research, detailed in *Nature Communications*, turned a previously identified noncovalent inhibitor of PLpro into a covalent one with higher potency, Parks said. Using mammalian cells, the team showed that the inhibitor molecule limits replication of the original SARS-CoV-2 virus strain as well as the Delta and Omicron variants.

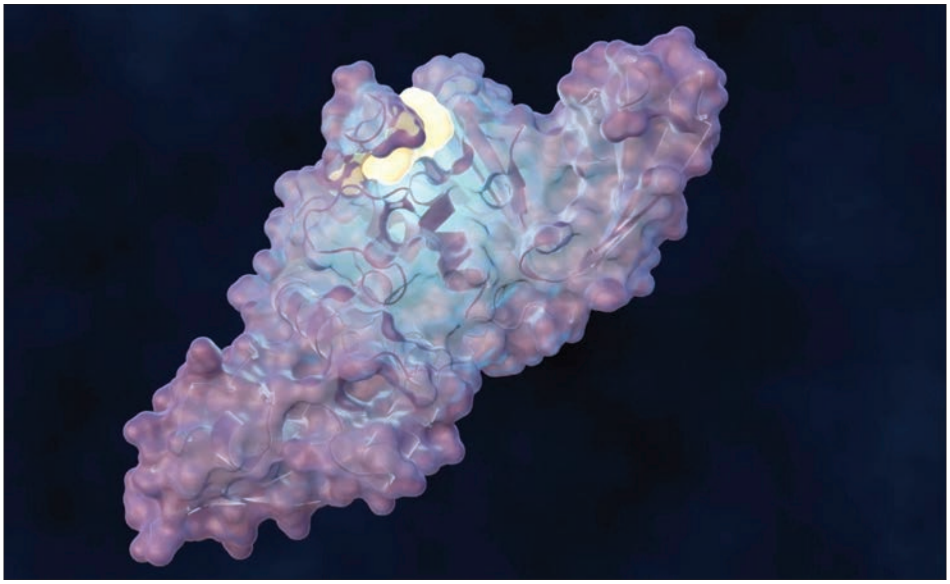
The ORNL scientists used computational modeling to predict whether their designs would effectively bind to the enzyme and disrupt its function. They then synthesized the molecules and tested them at ORNL and partner company Progenra to confirm their predictions.

The protein was expressed and purified using capabilities of the Center for Structural Molecular Biology at the Spallation Neutron Source at ORNL. The bright X-rays generated by the Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory were used to map the molecule and examine the binding process at an atomic level, validating the simulations. — *Stephanie Seay*

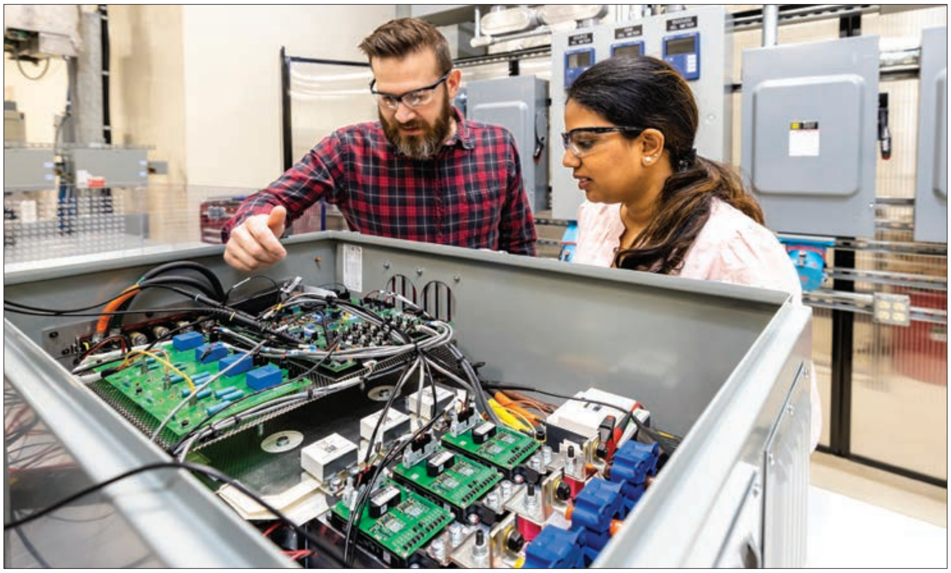
For more information: bit.ly/3nQhN1k

Electronics suite manages modern grid challenges

ORNL researchers are helping to modernize power management and enhance the reliability of an increasingly complex electric grid.



ORNL led a team of scientists to design a molecule that disrupts the infection mechanism of the SARS-CoV-2 coronavirus and could be used to develop new treatments for COVID-19 and future virus outbreaks.
Image credit: Michelle Lehman, ORNL



ORNL's Steven Campbell and Radha Krishna-Moorthy discuss part of the power electronics that make up the Smart Universal Power Electronics Regulator technology developed at ORNL. Image credit: Carlos Jones, ORNL

As the United States transitions to cleaner energy and more U.S. consumers adopt electric vehicles, the grid is facing new power flow demands. ORNL researchers are tackling this challenge by creating a new architecture to modernize the grid from the bottom up, starting with consumers and expanding to the entire power distribution system. A cornerstone of this architecture is a new power electronics technology suite called a Smart Universal Power Electronics Regulator, or SUPER.

The approach combines hardware and software to monitor equipment health, speed up communication and increase security. In the long run, that means fewer and shorter blackouts for customers, savings for utilities and a more reliable grid.

SUPER is a type of power converter consisting of "stackable" power electronics building blocks with enhanced abilities and intelligence. Just as the building blocks can be stacked within a SUPER system, the SUPER systems can also be stacked to make a data center, microgrid or electrical substation. To be universal, SUPER is designed with standardized interconnections and communication protocols, easing system integration for a wide range of applications.

Madhu Chinthavali, head of ORNL's Energy Systems Integration and Controls section, said this architecture can help manage clean energy both where it is generated and when it is transferred elsewhere through power lines. Today, that requires many pieces of equipment, which multiply grid connections, clutter grid communications and increase vulnerability to cyberattacks and electricity loss. SUPER can act as the gatekeeper between the grid and each power source or electrical load.

"The management of energy transfer is a big challenge, and ORNL is trying to build a structured partnership to accelerate the development of these concepts and potentially demonstrate them in the near term," Chinthavali said. ORNL has helped organize the Power electronics Accelerator Consortium for Electrification, or PACE, to quickly take innovations like SUPER to utilities and manufacturers. — *S. Heather Duncan*

For more information: bit.ly/3ZKAlgM

Proteins can help plants identify helpful microbes

ORNL researchers have identified specific proteins and amino acids that could control bioenergy plants' ability to identify beneficial microbes that can enhance plant growth and storage of carbon in soils.

These proteins, called LysM receptor-like kinases, regulate signaling between plants and microbes, a process that influences biomass production, root performance and carbon storage. The study showed these kinases potentially help poplar trees differentiate between helpful and disease-causing microbes.

One of the proteins identified through a new ORNL-developed approach could be key to communications between poplar trees and beneficial microbes that can help boost poplar trees' growth, carbon storage and climate resilience. Image credit: Andy Sproles, ORNL

With this information, scientists can better target bioengineering efforts aimed at promoting plant-microbe symbiosis to boost poplar trees' growth and sustainability in future climates.

"Having predictive insight into how receptors distinguish microbial friend from foe will reduce the number of design-build-test cycles needed to validate gene function and accelerate improvement of crop performance," said ORNL's Udaya Kalluri.

The novel method used computational structural biology in a multipronged approach that can accelerate gene function identification in a variety of plants. — *Kim Askey*

For more information:
https://bit.ly/3Kp91Pp

Mickey Wade to head fusion, fission directorate

Mickey Wade

Mickey Wade has been named associate laboratory director for ORNL's Fusion and Fission Energy and Science Directorate.

"To reach the nation's clean energy goals, we must develop and deploy nuclear energy technologies," said interim ORNL Director Jeff Smith. "Given his experience in industry and the national lab system, Mickey is the perfect choice to ensure ORNL is applying its leading expertise and capabilities to help the United States reach net zero."

In his new role, Wade will oversee the directorate's unique facilities, capabilities and skilled scientists and engineers who are tackling such challenges as extending operations of the current U.S. nuclear reactor fleet, investigating economical and flexible advanced reactor systems and making fusion energy a viable power source. The directorate leverages synergies between fusion and fission across domestic and international programs.

"The lab has a storied history in addressing compelling national challenges in energy, national security and environmental science through world-class research on harnessing atomic energy, neutron science, plasma physics and advanced nuclear technologies," Wade said. "The Fusion and Fission Energy and Science Directorate will continue this proud tradition of combining vibrant research programs, reliable facilities and cutting-edge expertise to accelerate the development of fusion and advanced fission energy systems."

Wade previously served in various leadership roles at General Atomics, including as the director of the DIII-D National Fusion Program. — *Sara Shoemaker*

Report sees opportunities to modernize hydropower

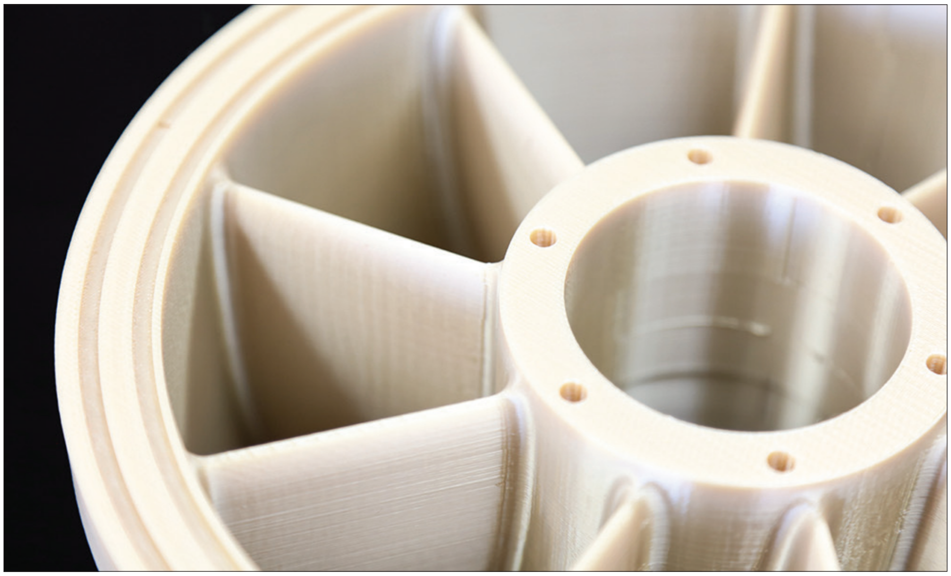
Over 100 years ago, the hydropower industry, which today generates 32 percent of all U.S. renewable energy, was built using traditional manufacturing processes. But surging energy demand, higher material costs and supply chain hurdles have led researchers to rethink the manufacturing of hydropower equipment.

A new report published by ORNL assessed how advanced manufacturing and materials, such as 3D printing and novel component coatings, could offer solutions to modernize the existing fleet and design new approaches to hydropower.

For the assessment, ORNL brought together representatives from the hydropower industry, advanced manufacturing industries, research institutions and groups committed to environmental stewardship.

Their collaboration identified existing infrastructure challenges and ways in which advanced manufacturing could enhance new design capabilities, improve system and component performance, reduce reliance on foreign manufacturing and better address environmental concerns.

"Hydropower has enormous potential in securing a cleaner, more sustainable



This newly manufactured fixed guide vane of a hydropower turbine system was printed at the DOE Manufacturing Demonstration Facility at ORNL. Image credit: Genevieve Martin, ORNL energy future," said ORNL's Mirko Musa. "We can build upon its success, layer by layer." — *Mimi McHale*

For more information: bit.ly/4370cCx

Chemist brings STEM to underserved youth

An ORNL chemist attracted national attention when her advocacy for science education made People magazine's annual "Women Changing the World" issue.

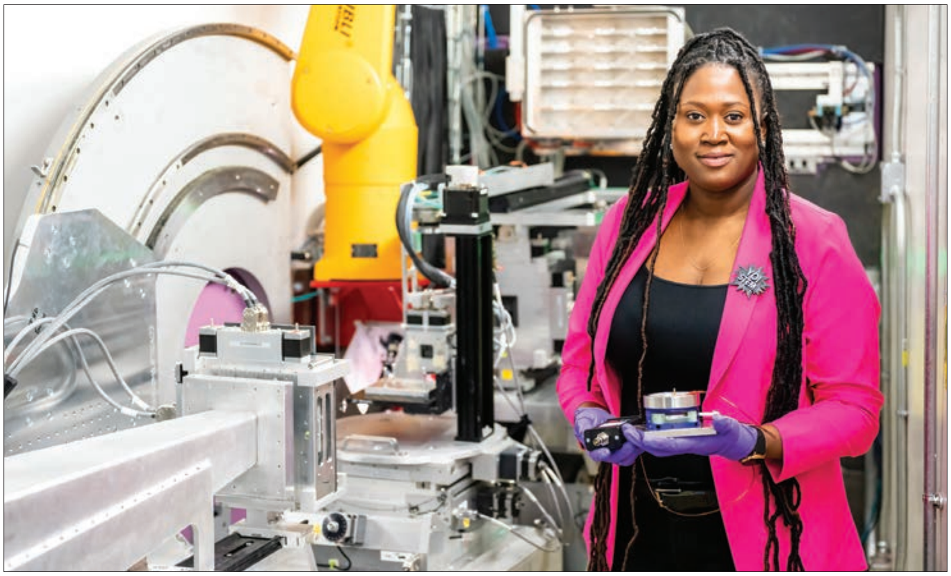
Seven years ago, Candice Halbert founded a nonprofit that connects diverse STEM professionals with underserved youth, including girls, cultural minorities, LGBTQ+ youth and kids from low-income families. YO-STEM, or Youth Outreach for Science, Technology, Engineering and Math, gives kids something Halbert did not get when she was young.

"A teacher once told me I thought like an engineer, but I didn't know what an engineer did," she said. "I thought they were train conductors. Had I known what a chemical engineer was earlier, I probably would have gone in that direction. YO-STEM gives kids the opportunity to learn about different types of science firsthand so they know what's possible."

Halbert envisions YO-STEM expanding into regional chapters, keeping the focus on students from underserved communities.

YO-STEM programming involves STEM professionals guiding youth through challenging scientific experiments, nurturing two vital ingredients for STEM success: critical thinking and collaboration. YO-STEM students experiment with different science- and engineering-based activities, such as genetic mutations in fruit flies, 3D printing, water quality testing and forensics — experiments the professionals might not have seen until college. — *Sumner Brown Gibbs*

For more information: http://bit.ly/43fzSWT



ORNL chemist and YO-STEM founder Candice Halbert at the Liquids Reflectometer at ORNL's Spallation Neutron Source. Image credit: Carlos Jones, ORNL

ORNL's Jeremy Busby to lead isotopes directorate

Jeremy Busby has been named associate laboratory director for ORNL's Isotope Science and Engineering Directorate.

"Jeremy is an accomplished leader with a considerable background in nuclear science and operations. These traits will help him successfully lead the laboratory's isotope and enrichment efforts, which are critical national missions," interim ORNL Director Jeff Smith said.

Jeremy Busby

Busby joined ORNL in 2004 and has served in several leadership roles at the laboratory, most recently as director of the Nuclear Energy and Fuel Cycle Division and associate lab director for the Fusion and Fission Energy and Science Directorate. Busby's strong attention to operational discipline and his deep understanding of nuclear science will ensure ISED's work is done safely and moves forward.

In his new role, Busby will lead a directorate of talented scientists and engineers charged with producing unique isotopes for various uses, developing enrichment technology and operating ORNL's nuclear facilities. The broad science portfolio for ISED includes making difficult-to-produce materials, such as actinium-225 for use in potential treatments for aggressive forms of cancer and plutonium-238 to power NASA's deep space missions.

"The lab has a proud history of delivering high-impact isotopes, positioning ORNL as a world leader in isotope research, development and production," Busby said. "ISED provides excellent stewardship of ORNL's nuclear and radiological facilities — the Radiochemical Engineering Development Center and numerous other hot cell facilities — that are critical in guiding the lab's efforts to broaden the application of isotopes for energy, environmental, medical and national security purposes. I'm honored to contribute to our success moving forward." — *Sara Shoemaker*

Exascale impact:

The Frontier supercomputer gets to work

by Katie Bethea and Matt Lakin
betheakl@ornl.gov

After debuting last year as ORNL's fourth No. 1 supercomputer in a row and granting access to its first users in April, Frontier settled into regular operations this summer.

Frontier is the first machine capable of exascale computing — one quintillion calculations per second — and researchers have already made breakthroughs in materials research, climate modeling and astrophysics.

"Frontier marks a sea change in computing and will allow us to tackle the world's most pressing scientific challenges," interim ORNL Director Jeff Smith said. "It was made possible by an intense collaborative effort among national laboratories, academic institutions and private industry to provide the hardware, applications and integration necessary to drive scientific discovery at the exascale."

Since the system's debut last year, ORNL staff have increased Frontier's performance by 92 petaflops — or 92 followed by 15 zeroes. If that added performance were a separate supercomputer, it would be the eighth fastest in the world.

Frontier features a theoretical peak performance of nearly 2 exaflops, or two quintillion calculations per second, making it 10 times more powerful than ORNL's Summit system, which was the world's fastest as recently as November 2019 and even now ranks fifth in the world. Frontier leverages ORNL's extensive expertise in accelerated computing and will enable scientists to

See INTRODUCING FRONTIER, page 10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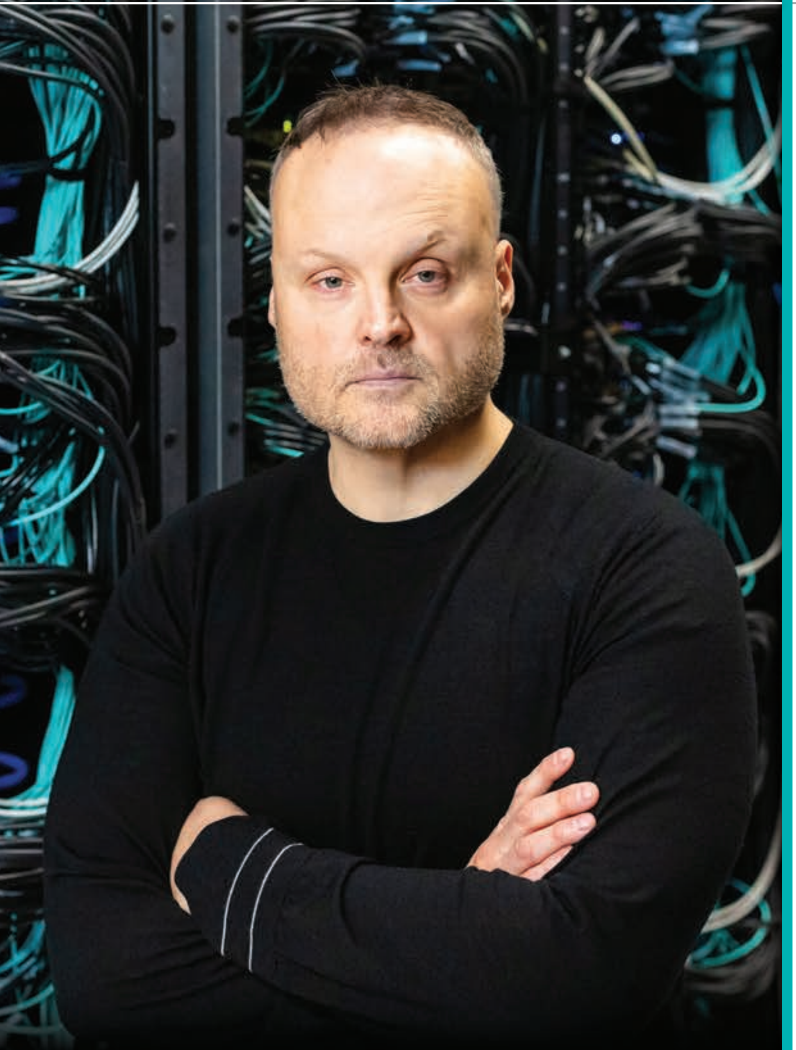


Frontier marks the start of the exascale era for scientific computing. The science that we're running on Frontier is going to ignite an explosion of innovation — and of new questions we haven't even thought of before.

— OLCF Director of Science **Bronson Messer**

INTRODUCING FRONTIER, page 8

develop critically needed technologies for the country's energy, economic and national security sectors, helping researchers tackle problems of national importance that were impossible to solve just five years ago.

As the world's most powerful AI machine, Frontier's novel architecture is also ideally suited for delivering unprecedented machine learning and data science insights and automations that could vastly improve our understanding of critical processes, from drug delivery to nuclear fusion to the global climate.

— Former ORNL Computing and Computational Sciences Associate Laboratory Director and Exascale Computing Project Director **Doug Kothe**

In addition to breaking the exascale barrier with a full-precision algorithm, Frontier's performance in mixed-precision computing — a much less demanding standard — clocked in at roughly 6.88 exaflops, or more than 6.8 quintillion calculations per second, as measured by the High-Performance Linpack-Accelerator Introspection, or HPL-AI, test. The HPL-AI test measures calculation speeds in the computing formats typically used by the machine learning methods that drive advances in artificial intelligence.

Detailed simulations traditional HPC users rely on to model such phenomena as cancer cells, supernovas, the coronavirus or the atomic structure of elements require 64-bit precision, a computationally demanding form of computing accuracy. Artificial intelligence and machine learning algorithms typically require much less precision — sometimes as little as 32-, 24- or 16-bit accuracy — and can take advantage of special hardware in the graphic processing units, or GPUs, relied on by machines like Frontier to reach their breathtaking speeds.

"As the world's most powerful AI machine, Frontier's novel architecture is also ideally suited for delivering unprecedented machine learning and data science insights and automations that could vastly improve our understanding of critical processes, from drug delivery to nuclear fusion to the global climate," said Doug Kothe, who until June was associate laboratory director of ORNL's Computing and Computational Sciences Directorate and director of the Exascale Computing Project.

Science on Day One

"Frontier marks the start of the exascale era for scientific computing," said OLCF Director of Science Bronson Messer. "The science that we're running on Frontier is going to ignite an explosion of innovation — and of new questions we haven't even thought of before."

ORNL scientific partners such as General Electric Aviation and GE Power have been among the first researchers to leverage the power of Frontier.

"GE Aerospace and Research is using exascale computing, including time on the Frontier supercomputer, to revolutionize the future of flight with sustainable hydrogen propulsion and hybrid electric technologies," said David Kepczynski, chief information officer at GE Research. "In pursuit of a net-zero carbon future, exascale supercomputing systems will be indispensable tools for GE researchers and engineers working at the cutting edge."

Frontier will also play a key role in climate science research because modeling climate phenomena is a challenging problem that brings researchers together from disciplines across the scientific arena. Staff members at ORNL will work with hospitals and the National Institutes of Health to draw connections between future climate data and human health data using the new supercomputer.

"With a computer like Frontier, we can take data out of climate models at very fine scales — at the county level of health," said Kate Evans, director of ORNL's Computational Sciences and Engineering Division. "For example, if you have hotter temperatures, you'll have more humidity, you'll have more ozone, and that affects the way we breathe."

Frontier will enable scientists to dive deeper into the nuances of the global climate, guiding them to new insights about how people live, move, work and adapt in a changing climate.

The Frontier system will also enable scientists to analyze health data more efficiently using artificial intelligence and machine learning techniques, leading to new understandings of disease processes and insights into possible drug targets. Researchers are working to train computers to read and understand chunks of medical records where patient information is often hidden. The CANcer Distributed Learning Environment initiative, or CANDLE, a joint endeavor led by DOE and the National Cancer Institute, focuses on developing language processing techniques to identify connections in patients' medical data.

"Exascale computing infrastructure, such as Frontier, will be the paradigm shift, because we can bring all of the data together and analyze it in a time-efficient way," said Gina Tourassi, director of the National Center for Computational Sciences at ORNL. "The end goal is to develop a general CANDLE library so that anyone with a deep learning code and a dataset can train their model at scale on a big HPC system without significantly modifying their code. We're also doing this in the context of DOE's partnership with the National Cancer Institute, so specific

See INTRODUCING FRONTIER, page 12

Facts about Frontier

The Frontier supercomputer includes some of the world's most advanced technologies from AMD and HPE.

- Each node contains one optimized third-generation AMD EPYC processor and four AMD Instinct MI250X accelerators for a systemwide total of 9,408 CPUs and 37,632 GPUs. These nodes provide developers with ease of programming for their applications owing to the coherency enabled by the processors and accelerators.
- HPE's Slingshot interconnect is the world's only high-performance Ethernet fabric designed for HPC and artificial intelligence. By connecting several core components (e.g., CPUs, GPUs, high-performance storage), Slingshot enables larger data-intensive workloads that would otherwise be bandwidth-limited and provides higher speed and congestion control to ensure applications run smoothly. Owing to this unique configuration and expanded performance, teams have taken a thoughtful approach to scaling the interconnect to a massive supercomputer such as Frontier, made up of 74 HPE Cray EX cabinets, to ensure reliable performance across applications.
- An input/output subsystem from HPE was brought online this year to support Frontier and the OLCF. The I/O subsystem features an in-system storage layer and Orion, which is a Lustre-based, enhanced centerwide file system. The in-system storage layer will employ compute-node local storage devices connected via PCIe Gen4 links to provide peak read speeds of more than 75 terabytes per second, peak write speeds of more than 35 terabytes per second and more than 15 billion random-read I/O operations per second. The Orion centerwide file system will provide around 700 petabytes of storage capacity and peak write speeds of 5 terabytes per second.
- As a next-generation supercomputing system and the world's fastest for open science, Frontier is also liquid cooled. This cooling system promotes a quieter data center by removing the need for a noisier, air-cooled system.

This project marks the culmination of more than three years of effort by hundreds of dedicated ORNL professionals and their counterparts at HPE and AMD and across the DOE community. Their hard work will enable scientists around the world to begin their explorations on Frontier. At the OLCF, we're proud of our legacy of world-leading computer excellence.

— Former OLCF Program Director **Justin Whitt**

INTRODUCING FRONTIER, page 11

deep learning models that we are developing are focused on cancer research and precision medicine challenges."

In the same vein, Frontier will enable researchers to understand how seismic activity affects the structural integrity of buildings and infrastructure, and ultimately to predict earthquake damage at the building level.

As the world's first exascale supercomputer and the world's largest system for AI, Frontier has already demonstrated its powerful innovation in driving scientific breakthroughs that were previously impossible, in aerodynamics, climate, medicine and nuclear physics. We are proud of our continued collaboration on Frontier with Oak Ridge National Laboratory and look forward to future discoveries the system will unlock.

— President and CEO of Hewlett Packard Enterprise **Antonio Neri**

Today, building-level earthquake risks are extrapolated from the limited data of past major seismic events. Small-scale models and historical observations are helpful, but they don't tell the whole story of the impacts of a geological event as powerful and far-reaching as a major earthquake.

"Our goal is to advance the state of computational capabilities so we can model all the way from the fault rupture to the waves propagating through the earth to the waves interacting with the structure," said Lawrence Berkeley National Laboratory senior scientist David McCallen, principal investigator for the EQSIM application.

"We're doing things now that we only thought about doing a decade ago, like resolving high-frequency ground motions. It is really an exciting time for those of us who are working on simulating earthquakes."

It takes a village

The work to deliver, install and test Frontier began in the midst of the COVID-19 pandemic, as shutdowns around the world strained international supply chains. More than 100 team members worked around the clock to source millions of components, ensure timely deliveries of system parts and carefully install and test 74 HPE Cray EX cabinets that include more than 9,400 AMD-powered nodes and 90 miles of interconnect cables.

"As the world's first exascale supercomputer and the world's largest system for AI, Frontier has already demonstrated its powerful innovation in driving scientific breakthroughs that were previously impossible, in aerodynamics, climate, medicine and nuclear physics," said Antonio Neri, president and CEO of Hewlett Packard Enterprise. "We are proud of our continued collaboration on Frontier with Oak Ridge National Laboratory and look forward to future discoveries the system will unlock."

Each of Frontier's more than 9,400 nodes is equipped with a third-generation AMD EPYC CPU and four AMD Instinct MI250X GPUs. Combining traditional CPUs with GPUs to accelerate the performance of leadership-class scientific supercomputers exemplifies the hybrid computing paradigm pioneered by ORNL and its partners.

"At its heart, Frontier highlights the importance of long-term public–private partnerships and the important role high-performance computing plays in advancing scientific research and national security," said Lisa Su, chair and CEO of AMD. "I am excited to see Frontier enable large-scale science research that was previously not possible, leading to new discoveries that will transform our daily lives."

Frontier's deployment adds to ORNL's nearly 20-year tradition of supercomputing excellence alongside predecessors Jaguar, Titan and Summit — each the world's fastest computer in its time.

"This project marks the culmination of more than three years of effort by hundreds of dedicated ORNL professionals and their counterparts at HPE and AMD and across the DOE community," said Justin Whitt, who until June 2023 was program director of the OLCF. "Their hard work will enable scientists around the world to begin their explorations on Frontier. At the OLCF, we're proud of our legacy of world-leading computer excellence."

Frontier also ranks second on the Green500 list, which rates a supercomputer's energy efficiency in terms of performance per watt. Frontier clocked in at 62.68 gigaflops, or nearly 63 billion calculations, per watt.

The Frontier team has fine-tuned the system's performance as part of the scheduled acceptance testing process. Research teams prepared their scientific codes for the system so that they could run during the early system access period, and users selected through DOE's Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, and Advanced Scientific Computing Research Leadership Computing Challenge, or ALCC, programs now have access to Frontier.

Frontier supports many of the same compilers, programming models and tools that have been available to OLCF users on ORNL's Titan and Summit supercomputers. Summit has been a premier development platform for Frontier and now will continue operating in tandem with the new system.

"We worked really hard to be ready for science on Day One, and we were," said Ashley Barker, head of the OLCF's Operations Section. "We have more than 1,200 users running on Frontier, and we're already seeing ground-breaking science achievements."

"

Exascale computing infrastructure, such as Frontier, will be the paradigm shift, because we can bring all of the data together and analyze it in a time-efficient way.

— ORNL National Center for Computational Sciences Director **Gina Tourassi**

ORNL's methodical leap into the exascale era

by Coury Turczyn
turczyncz@ornl.gov

With the May 2022 launch of Frontier, ORNL officially vaulted the United States into the exascale era of high-performance computing. But back in 2008, the feasibility of exascale machines that can perform a billion billion floating point operations per second looked bleak.

The University of Notre Dame's Peter M. Kogge led a study sponsored by the Defense Advanced Research Projects Agency to identify exascale's key hurdles. Published in May 2008, *Technology Challenges in Achieving Exascale Systems* surveyed HPC experts from universities, research labs and industry to predict whether the nation could — by 2015 — attain a thousandfold increase in computational power over then-new petascale systems.

Their consensus? Not without changing the trajectory of HPC technology from the state of the art at that time.

But now, 15 years later, exascale computing has become a reality, albeit not quite as soon as DARPA had hoped. Frontier is the harbinger of a new era in computational science, to be followed in the next few years by Aurora at Argonne National Laboratory and El Capitan at Lawrence Livermore National Laboratory. These exascale supercomputers will tackle more extensive problems and answer more complex questions than ever before.

How did the Oak Ridge Leadership Computing Facility and its vendor partners AMD and HPE Cray overcome the obstacles identified in Kogge's report? It took a lot of organizational work, several false starts and some fortuitous advances in computing technology.

"We had to build more energy-efficient processors. We had to build more reliable hardware and better interconnects. We had to be able to move data around more efficiently. We had to design algorithms that can use that level of concurrency," said Jack Dongarra, until recently the director of University of Tennessee, Knoxville's Innovative Computing Laboratory. Concurrency is the ability to process more than one task at the same time, with no two tasks executing at the same instant.

"Those are all complicated things, and it required research to develop the technology necessary to achieve them. But in the intervening 10 years or so, we did just that," Dongarra said.

Planning ahead for a new class of supercomputer

To design and construct a next-generation supercomputer, the first step is the trickiest: finding funding. But to convince government agencies — and, in turn, Congress — to spend large sums on cutting-edge technology, a strong case must be made for its necessity and feasibility, and that entails lots of study groups and a lot of effort to find consensus.

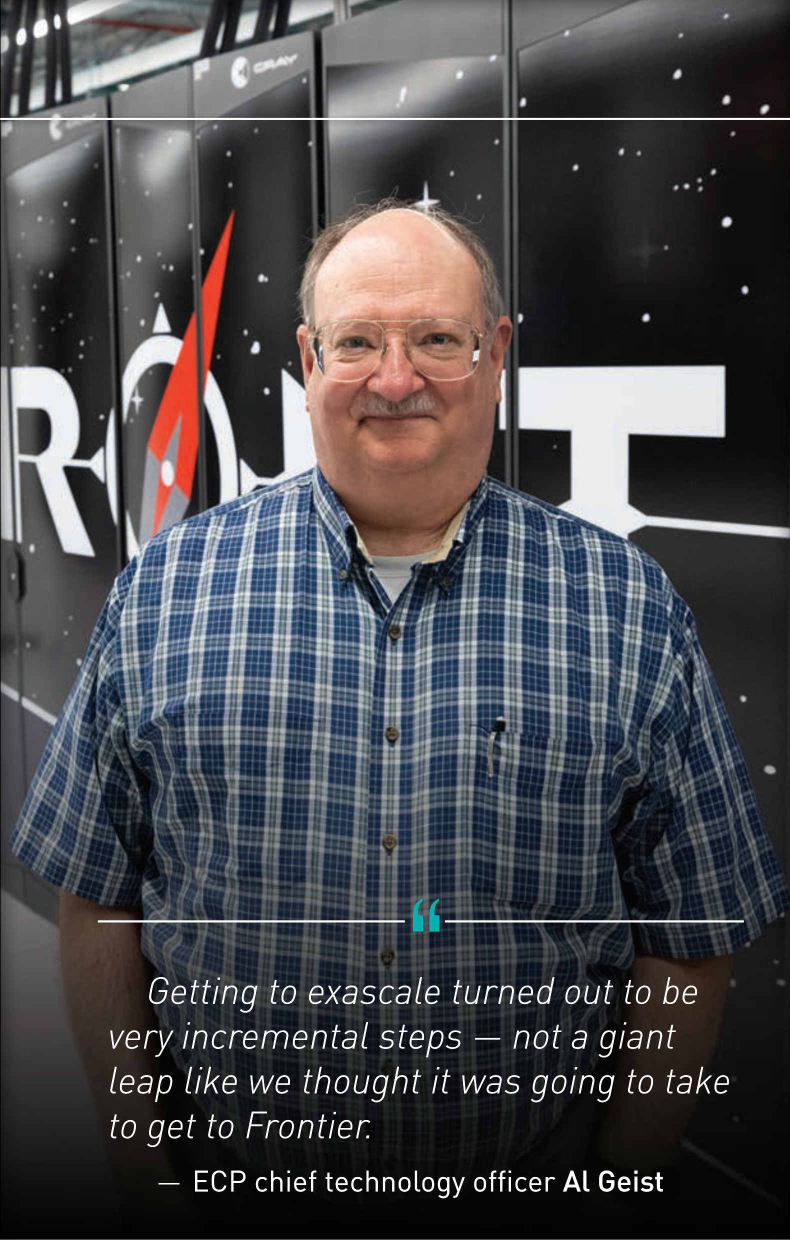
Many reports were published in the decade following that first exascale study, usually with Dongarra's name on them. Many examined the possibilities — and potential impossibilities — of exascale computing. Most identified the same two technical challenges that needed to be overcome to achieve exascale: reducing energy consumption and increasing the reliability of the chips powering these massive systems.

Meanwhile, exascale alliances between the national labs began forming with the goal of figuring out how to solve those technical challenges — and of gaining enough political traction to move exascale projects through federal agencies. Most fizzled, but forward motion toward exascale came on three fronts.

First, relationships with computer technology vendors were formalized in 2012 with DOE's FastForward and DesignForward programs. FastForward focused on the processor, memory and storage vendors — such as AMD and Intel — to address power consumption and resiliency issues. DesignForward focused mainly on system integrators such as HPE, Cray and IBM to plan packaging, integration and engineering. Cray was later acquired by HPE, in 2019.

Second, the Collaboration of Oak Ridge, Argonne, and Livermore, or CORAL, was formed by DOE in 2012 to streamline the supercomputer procurement process. Each lab was acquiring pre-exascale systems at the time, and it made sense for them to work together. CORAL-2 continues this successful collaboration with the goal of procuring exascale systems.

Third, the Exascale Computing Project launched in 2016 as part of DOE's Exascale Computing Initiative, assembling over 1,000 researchers from 15 labs, 70 universities and 32 vendors to tackle exascale application development as well as software libraries and software technologies. The software will be a critical factor in determining the early success of the new exascale systems.



Getting to exascale turned out to be very incremental steps — not a giant leap like we thought it was going to take to get to Frontier.

— ECP chief technology officer **Al Geist**

"We are very fortunate to have access to a one-of-a-kind, world-class supercomputer, and we don't want to let it sit idle for even a single minute. We are delivering a wide range of applications and software technologies that can use this precious resource to solve problems of national interest," said Lori Diachin, ECP project director and deputy associate director for science and technology in LLNL's Computation Directorate.

"Everything has to be production-hardened quality, performant and portable on Day One. So, to get the largest return on taxpayer investment, and the fastest route to new scientific discovery, we have to have all these apps ready."

With these programs in place, requirements for actual exascale systems needed to be solidified for DOE to issue Requests for Information and Requests for Proposals, necessary steps in the government procurement process to spur competition between vendors.

"We need these machines to be stable so that, in concert with our apps and software stack, they can fulfill their promise of being consequential science and engineering instruments for the nation," said Doug Kothe, former associate laboratory director of ORNL's Computing and Computational Sciences Directorate, who was replaced as ECP director by Diachin in 2023. "So, we as a community started talking about this years ago — and talking means writing down answers to key requirements questions like: Why? What? How? How well? What do we need to focus on in terms of R&D and software?"

Many of those questions revolved around what basic architecture the system would ultimately use — which was partly determined by a choice made by the OLCF years earlier to use a piece of consumer PC hardware in supercomputers.

Specifying the future of HPC

Before the OLCF's Titan debuted in 2012, graphics processing units, or GPUs, were best known for powering high-end gaming PCs. At the time, most supercomputers relied only on central processing units, or CPUs, to crunch their algorithms. But Titan introduced a revolutionary hybrid processor architecture that combined AMD 16-core Opteron CPUs and NVIDIA Kepler GPUs, which tackled computationally intensive math problems. At the same time, the CPUs efficiently directed tasks, thereby significantly speeding up calculations.

"Titan's GPU-based system was a unique supercomputer design at the time," Kothe said. "I don't think the whole community bought into it or thought it would become the base technology for exascale. Oak Ridge believed that accelerated-node computing would be the norm for the foreseeable future, and so far that has come to fruition."

Titan led to many more GPU-based supercomputers, including Summit in 2017 — Titan's successor at the OLCF — and LLNL's Sierra in 2018. They both employ NVIDIA V100 GPUs, and that choice also proved important in configuring the upcoming exascale system's capabilities.

Al Geist, chief technology officer for the ECP and the OLCF, wrote many of the documents for CORAL and CORAL-2. He sees Summit's architecture as another fortunate turning point in supercomputer design.

"As supercomputers got larger and larger, we expected them to be more specialized and limited to a small number of applications that could exploit their particular capabilities. But what happened when Summit was announced, NVIDIA jumped up and said, 'Oh, by the way, those Volta GPUs have something called tensor cores in them that allow you to do AI calculations and all sorts of additional things,'" Geist said. "They could do the traditional HPC modeling and simulation, but Summit is also very effective at doing high-performance data analytics and artificial intelligence."

The ability of GPUs to greatly accelerate performance as well as handle mixed-precision math for data science — all while using less power than CPUs — made them the best choice for exascale architecture, especially with more powerful and efficient next-generation chip designs being produced by vendor partners like AMD, Intel and NVIDIA.

"What we found out in the end is that exascale didn't require this exotic technology that came out of that 2008 report," Geist said. "We didn't need special architectures. We didn't need new programming paradigms. Getting to exascale turned out to be very incremental steps — not a giant leap like we thought it was going to take to get to Frontier."

Exascale tools for developing new reactors

by Coury Turczyn
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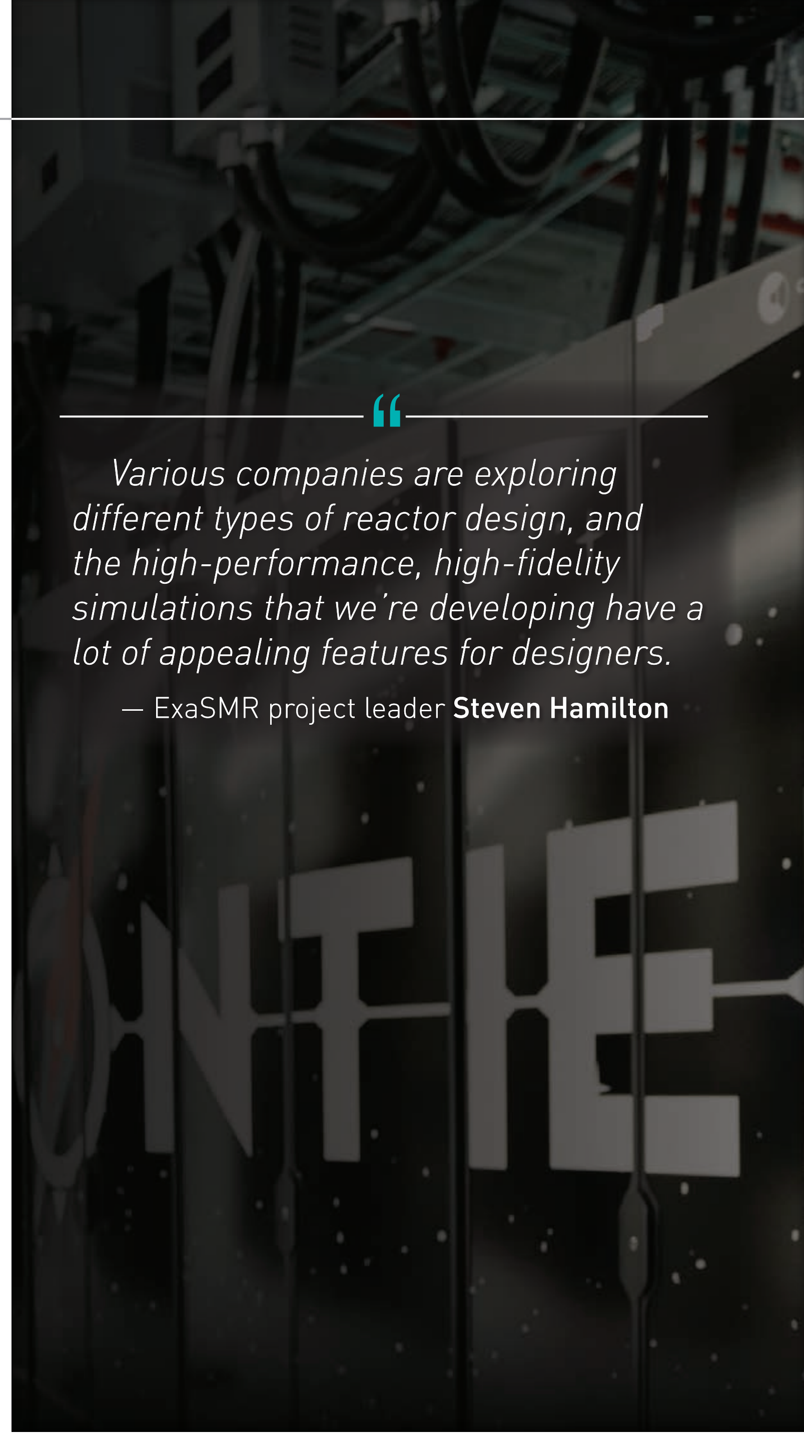
As renewable sources of energy such as wind and sun power are increasingly added to the country's electrical grid, old-fashioned nuclear energy is also being primed for a resurgence.

For the past 20 years, fission reactors have produced a nearly unchanging portion of the nation's electricity: around 20 percent. But that percentage could start increasing soon. The advent of small modular reactors, or SMRs, and advanced reactor concepts, or ARCs, signals a new generation of fission power. SMRs are substantially smaller than most commercial nuclear reactors today, and they use standardized designs, thus reducing construction costs and production time. Meanwhile, ARCs explore new technologies to produce fission power more efficiently and safely.

Exascale Small Modular Reactor, or ExaSMR, is a suite of exascale-optimized simulation codes that aims to provide the nuclear industry's engineers with the highest-resolution simulations of reactors to date and, in turn, help advance fission power. Supported by DOE's Exascale Computing Project since 2016, the ExaSMR project endeavors to leverage the next-generation power of exascale supercomputers — capable of at least a quintillion calculations per second — to make large-scale nuclear reactor simulations easier to access, cheaper to run, and more accurate than the current state of the art.



> *Various companies are exploring different types of reactor design, and the high-performance, high-fidelity simulations that we're developing have a lot of appealing features for designers.*
>
> — ExaSMR project leader **Steven Hamilton**

ExaSMR's performance on ORNL's Frontier supercomputer — an HPE Cray exascale system currently ranked fastest in the world — showed a 100 times speedup of its codes compared to baseline simulations performed on Titan, the U.S.'s most powerful supercomputer in 2016. That's when ECP set out to develop advanced software for the arrival of exascale-class supercomputers, which occurred with Frontier's debut in 2022.

"By accurately predicting the nuclear reactor fuel cycle, ExaSMR reduces the number of physical experiments that reactor designers would perform to justify fuel use," said ExaSMR project leader Steven Hamilton. "In large part, that's what simulation is buying companies: a predictive capability that tells you how certain features will perform so that you don't need to physically construct or perform as many experiments, which are enormously expensive."

Coupling physics codes

Commercial nuclear reactors generate electricity by splitting uranium nuclei to release energy in a process known as fission. This energy turns water into steam, which spins electricity-producing turbines. ExaSMR integrates the most accurate computer codes available for modeling the physics of this operation, creating a toolkit that can predict a reactor design's entire fission process. The toolkit includes the Shift and OpenMC codes for neutron particle transport and reactor fuel depletion and the NekRS code for thermal fluid dynamics.

Although most of these codes are already well established in science and industry, the ExaSMR team has given them a complete exascale makeover. For the past seven years, researchers from ORNL, Argonne National Laboratory, the Massachusetts Institute of Technology and Pennsylvania State University have been optimizing the codes for exascale supercomputers such as Frontier and Argonne's forthcoming Aurora.

"What we're doing in ExaSMR is a coupled physics simulation between the neutron transport and the fluid dynamics — these two physics codes talk back and forth," said Hamilton, an R&D scientist in ORNL's HPC Methods for Nuclear Applications group.

"The neutron transport is telling you where the heat is generated. That heat becomes a source term for the fluid dynamics calculation. The fluid dynamics calculates the temperature resulting from that heat source. And then you can adjust the parameters in the simulation until the neutron transport and the fluid dynamics are in agreement."

ExaSMR's ability to accurately model in high resolution the whole reactor process — the amount of heat produced by nuclear fission, the ability of the reactor to transfer that heat to power generators, and the life expectancy of the entire system — provides engineers with key insights to ensure the safety and efficiency of their reactor designs.

What's ahead for ExaSMR?

Partnering with Westinghouse, a producer of commercial nuclear power technology, the ExaSMR team applied for a Leadership Computing Challenge grant from DOE's Office of Advanced Scientific Computing Research. Westinghouse wants to evaluate the impact of using fuel enriched to higher levels of fissile uranium-235 than that currently used in its reactors. Running ExaSMR on Frontier will allow the company to perform high-fidelity simulations to predict how different types of fuels would perform if used in an operating reactor.

Likewise, Hamilton wants to apply ExaSMR to current ARC technologies being explored in the power industry. The DOE Office of Nuclear Energy's Advanced Reactor Demonstration Program provides funding for commercial companies to accelerate the demonstration of advanced reactors. Two such reactors are slated for near-term deployment by 2027: X-energy's Xe-100 pebble-bed reactor and TerraPower's Natrium sodium-cooled fast reactor. Five additional designs from Kairos, Westinghouse, BWX Technologies, Holtec International and Southern Company are ramping up for longer-term deployment.

Hamilton foresees ExaSMR becoming an indispensable tool for companies entering a new era of nuclear power.

"Various companies are exploring different types of reactor design, and the high-performance, high-fidelity simulations that we're developing have a lot of appealing features for designers," he said. "It's unlikely, in the near future, that we'll have enough confidence in simulations that they would fully replace experiments, but if we can reduce the number of experiments that are performed, then there can be huge gains for these companies."

OLCF teams fine-tune Frontier for science

by Matt Lakin
lakinmn@ornl.gov

The world's first exascale supercomputer rocked the computing world with record speeds last year, but Frontier fully opened for scientific business only in 2023.

The HPE Cray system shot to No. 1 on the TOP500 list of the world's fastest supercomputers in May 2022 with a record speed of 1.1 exaflops, or 1 quintillion calculations per second, capping more than a decade of work to break the exascale barrier. But that announcement didn't mean the job was done.

Work continued through the second half of the year, led by the Oak Ridge Leadership Computing Facility's scientific engagement and user acceptance experts, to certify that Frontier met all the standards to enable the world-changing discoveries promised by exascale.

"There have been a lot of people involved, and it's been a long process, especially for all the users eager to start running their projects," said Ashley Barker, who oversees the OLCF's Operations Section. "Everyone wants to know when they can get on Frontier, so our lives became a little more exciting at year's end than when we started some of this work. But the time we spent testing on the front end will minimize any suffering later. We had to make sure the network would be stable and everything would run smoothly."

Ensuring Frontier runs as advertised spanned two fronts: the hardware and software, handled mainly by the Operations Section, and the codes developed to run the various simulations, handled mainly by the Scientific Engagement Section. Some codes had

From left, System Acceptance and User Environment Group Leader Verónica Melesse Vergara; Operations Section Head Ashley Barker; User Access, Outreach, and Communication Group Leader Katie Bethea; and User Assistance Group Leader Chris Fuson. Image credit: Carlos Jones, ORNL

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>
> — OLCF Operations Section Head **Ashley Barker**

already been run on Summit, Frontier's predecessor, and most have also been run on Crusher, the prototype system for Frontier — equivalent to about one-and-a-half of Frontier's 74 cabinets, or 192 of its more than 9,400 nodes — by codes teams working with users at the OLCF's Center for Accelerated Application Readiness.

"It's a big difference from how the changeover was handled with previous systems," said Verónica Melesse Vergara, who leads the System Acceptance and User Environment Group. "On Summit, we never had any real outside users on the system until it opened. This way we had more time to try everything out and uncover errors we could fix before the final unveiling. Early on is always the time to find those errors, because otherwise we'd be finding them while people are running projects."

Those projects range from national security challenges to probing renewable energy sources to fundamental questions of physics, chemistry, biology and astronomy. Some rely on new codes made to order, others on codes that date back to the first generation of supercomputers.

"We're always looking to improve performance," said Matt Norman, who leads the Advanced Computing for Life Sciences and Engineering Group. "Some codes have been ported across machines for decades and may do fine but need a boost. On some teams, our experts are almost part of the study as we work with the principal investigators to help them understand what kind of scientific approach will get the best performance."

The codes powering those studies can run to millions of lines of complex equations, intended to simulate scenarios like functioning windmills, nuclear reactions and exploding stars. The shift to Frontier involved some major changes in programming language that called for alterations.

"These codes are like information pipelines," said Dayle Smith, who leads the Advanced Computing for Chemistry and Materials Group. "The equations are like interlocking segments working together, so we couldn't necessarily just swap one part out for another. There can be a challenge adjusting what worked well on Summit to run even better on Frontier."

Rewriting an established code from scratch tends to be the least-preferred option.

"It's an iterative process," said Tom Beck, who oversees scientific engagement. "Our experts offer guidance to the vendors and users on potential tweaks and trade-offs. This work will be crucial to get their studies up and running, now and in the future."

As 2022 wound down, the finish line came into sight.

"It's been a long road, but we were always optimistic," Vergara said. "There were just so many nodes to test. Now that we've finished the tests, we hope the users will find it worth the wait. We've cleared the path so they can work at top speed."

Pioneering Frontier

Here are a few of the many talented ORNL employees behind the construction and operation of Frontier.

Denise Hoomes

Project Controls Lead

Denise Hoomes has always enjoyed puzzles. Today, Hoomes works on puzzles related to the nation's first exascale supercomputer, leading the project controls specialists working on the Frontier supercomputer project. In her role, she pieces together information about schedule, scope and budget for the fastest supercomputer in the world.

"Oftentimes, there are a multitude of ways to solve a problem," Hoomes said. "When we get the project controls team and the risk team and the technical leads together, we can bounce ideas off one another."

Rick Griffin

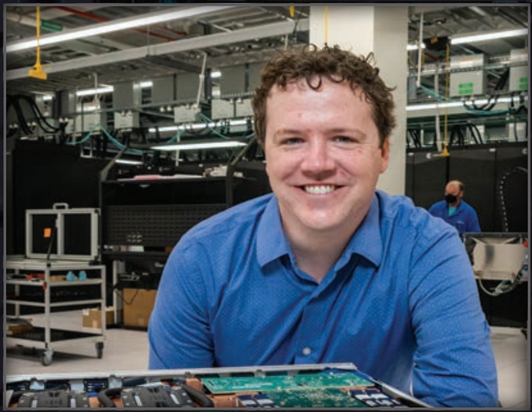
Electrical Engineer

Charged with helping install over 15 systems at ORNL, Rick Griffin is highly experienced with getting power safely and reliably to the world's most advanced supercomputers. His 30-megawatt masterpiece of electrical design is the OLCF's Frontier system.

"Frontier is the culmination of 20 years of experience with supercomputer electrical infrastructure," Griffin said. "With every new system, we learn something we can apply to the next system."

Matt Ezell

HPC Systems Engineer

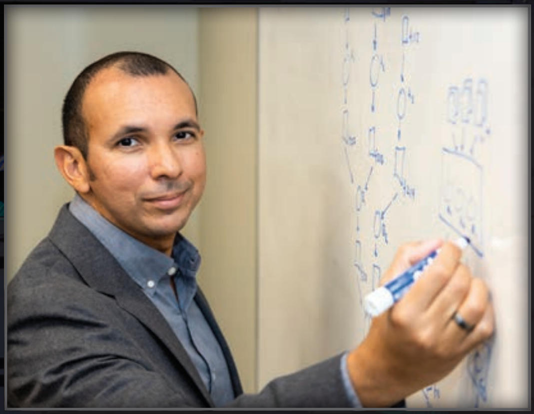


The system lead for Frontier, Matt Ezell, and his team met on a near-daily basis in coordination with the system vendor, HPE, to set up and optimize the system. Once all the hardware for Frontier had arrived in late 2021, his team began diligently working to ensure that Frontier will run smoothly and efficiently.

"At the end of the day, the project team is going to ask me specifically how things are going," Ezell said. "But that doesn't mean there's not a whole host of people working on this. It takes an army — a village — to raise a system."

Rafael Ferreira da Silva

Senior R&D Scientist, Scientific Workflows



Rafael Ferreira da Silva's job is to make life simple — at least for the thousands of users who access the OLCF's computing resources each year. That's because Ferreira da Silva, a senior R&D scientist in the National Center for Computational Sciences, works on the design and deployment of scientific workflow applications and tools used on OLCF supercomputers, an important part of the user experience and success on Frontier.

"We are part of the Advanced Technologies Section at ORNL, so we are thinking about the future, and the future is Frontier," Ferreira da Silva said. "The goal is trying to think ahead and not be deploying software as the users come on, but to have the software available already."

John Gounley

Computational Scientist

Without scientific codes that scale, exascale would be little more than a number. That's why computational scientists are working hard to ensure their codes run on exascale supercomputers as soon as these systems come online. John Gounley is working on codes for the CANcer Distributed Learning Environment project, which will provide deep learning methodologies to accelerate cancer research on exascale machines like Frontier.

"I work on the high-performance computing side of projects," Gounley said. "I help take things we've done at small scales and get them up and running on big leadership computing systems like Frontier."

Suzy Tichenor

Industrial Partnerships Director

From companies building the most powerful jet engines to ones developing new autonomous vehicles, Suzy Tichenor works to build trust relationships and help them apply for computing time on the OLCF's systems, including Frontier.

"These companies are passionate about their work, and their results touch our lives in so many ways that we don't realize. It's very gratifying to help them gain access to our leadership systems and the expertise of our world-class researchers so they can meet their goals and dreams."

Quantifying qudits:

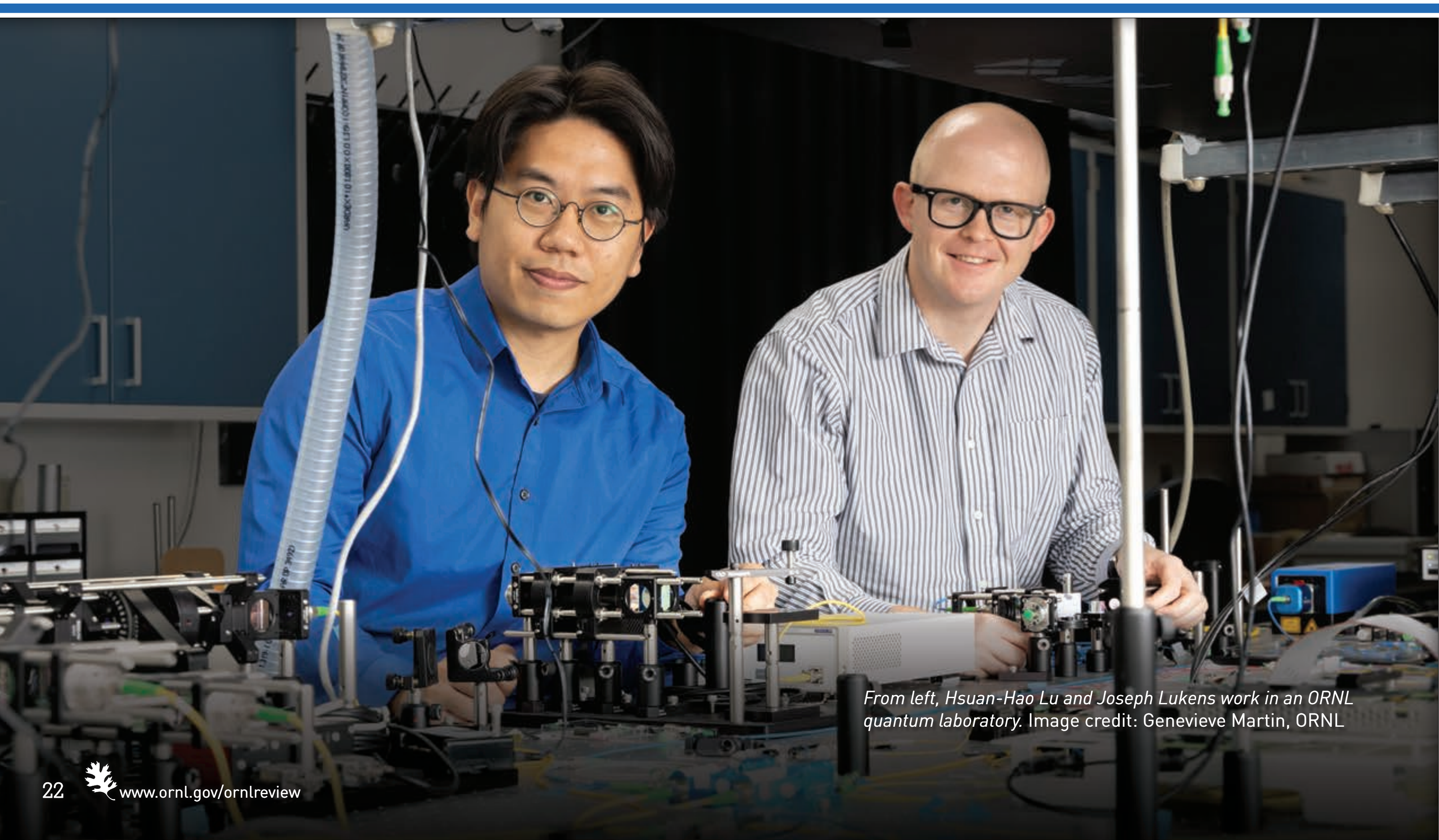
Measurements provide glimpse of quantum future

By Elizabeth Rosenthal
rosenthalec@ornl.gov

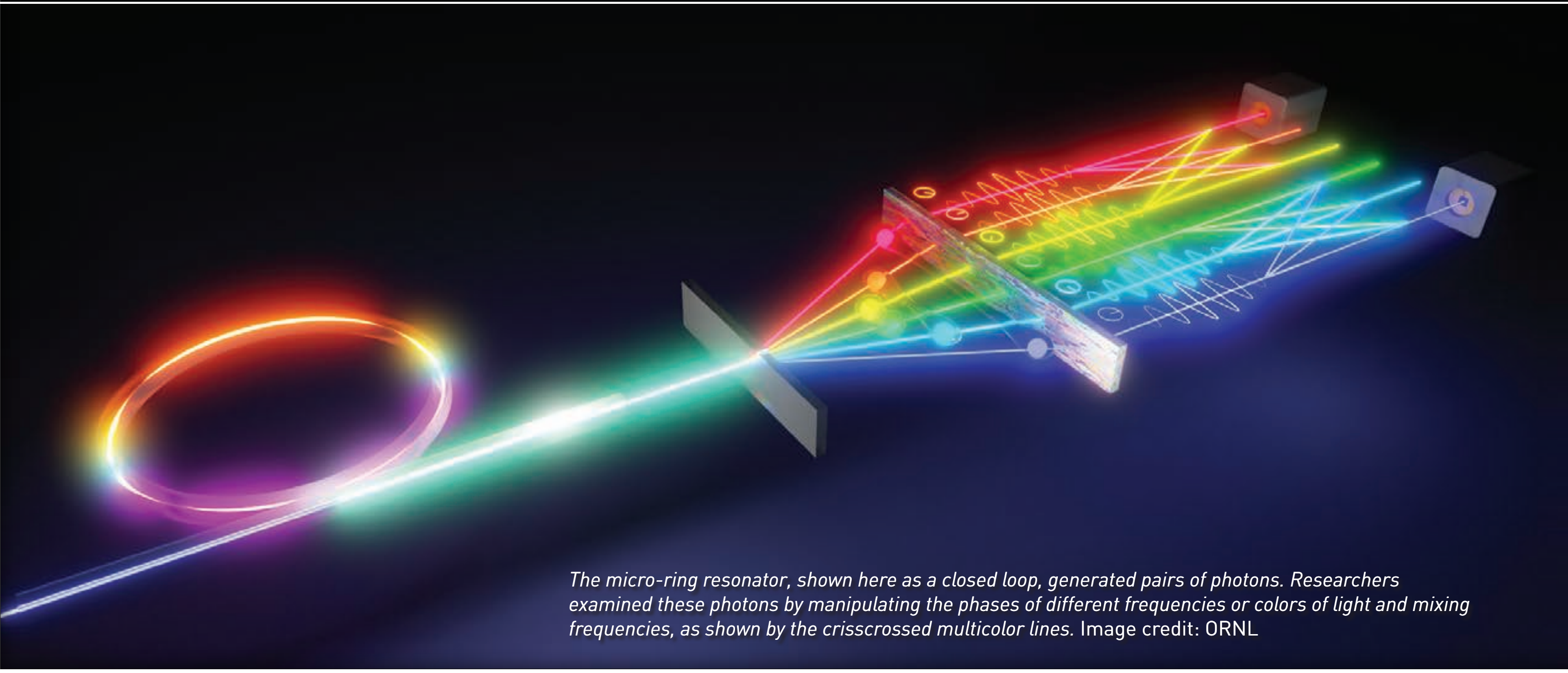
The word "qudit" might look like a typo, but this lesser known cousin of the qubit, or quantum bit, can carry more information and is more resistant to noise. These qualities are invaluable for improving the performance of quantum key distribution systems, quantum networks and, eventually, the quantum internet.

The "d" in qudit stands for the number of dimensions that can be encoded into a photon. Quantum bits with two dimensions are considered standard qubits, whereas those with three or more are called qudits. The more dimensions a qudit has, the more information it can carry for quantum applications.

To more accurately measure the quality of qudits encoded in photons produced by sources on an optical chip, researchers from ORNL, Purdue University and the Swiss Federal Institute of Technology Lausanne, or EPFL, developed an improved method for measurement that works at higher dimensions than previously possible. These measurements are essential for confirming that



From left, Hsuan-Hao Lu and Joseph Lukens work in an ORNL quantum laboratory. Image credit: Genevieve Martin, ORNL



The micro-ring resonator, shown here as a closed loop, generated pairs of photons. Researchers examined these photons by manipulating the phases of different frequencies or colors of light and mixing frequencies, as shown by the crisscrossed multicolor lines. Image credit: ORNL

the qudits are usable for future quantum information processing experiments.

Qudits are especially difficult to measure when they are entangled, meaning that measurements on one qudit can influence measurements on another qudit, regardless of the physical distance between them. Despite this added challenge, the researchers' method allowed them to fully characterize an entangled pair of qudits, each containing eight separate dimensions and together forming a quantum space containing 64 dimensions — quadrupling the previous record for discrete frequency modes. These results were published in *Nature Communications*.

"We've always known that it's possible to encode qudits with 10 or 20 dimensions or even higher using the colors of photons, or optical frequencies, but the problem is that measuring these particles is very difficult," said Hsuan-Hao Lu, a postdoctoral research associate at ORNL.

The researchers began their experiments by shining a laser into a micro-ring resonator — a circular on-chip device fabricated by EPFL and designed to generate entangled photons. Using this powerful photon source, which is comparable in size to the point of a sharpened pencil, the team generated frequency bin pairs — two qudits in the form of photons that are entangled in their frequencies.

> *We used our technique to characterize qudit entanglement with a level of precision that hasn't been shown before.*
>
> — Senior director of quantum networking at Arizona State University **Joseph Lukens**

"We used our technique to characterize qudit entanglement with a level of precision that hasn't been shown before," said Joseph Lukens, senior director of quantum networking at Arizona State University, who has a joint faculty appointment at ORNL.

The researchers used optical devices, including an electro-optic phase modulator that mixed different frequencies of a light, and a pulse shaper that modified the phase, or relative timing, of those frequencies. They performed these operations randomly to capture various frequency correlations, which Lu compared to rolling a pair of six-sided dice and recording how many times each combination of numbers appears — but in this case, the dice are entangled.

"This technique is pursued in the classical context for ultrafast and broadband photonic signal processing and has been extended to the quantum avenue of frequency qudits," said Andrew Weiner, who leads Purdue's Ultrafast Optics and Optical Fiber Communications Laboratory, where Lu studied before joining ORNL.

To infer which quantum states produced frequency correlations ideal for qudit applications, the researchers developed a data analysis tool based on a statistical method called Bayesian inference and ran computer simulations at ORNL.

Karthik Myilswamy, a graduate student at Purdue, plans to bring the micro-ring resonator to ORNL so the team can test quantum communication protocols such as teleportation — a method of transporting quantum information — and entanglement swapping — the process of entangling two previously unrelated particles — on the laboratory's quantum local area network.

"Now that we have a method to efficiently characterize entangled frequency qudits, we can perform other application-oriented experiments," Myilswamy said.

Cell membrane discovery

heralds computing advances

by Emily Tomlin
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While studying how bio-inspired materials might inform the design of next-generation computers, scientists at ORNL achieved an unprecedented result: the first identified nanoscale structure in which memory can be encoded.

The team explains in the *Proceedings of the National Academy of Sciences* how an artificial cell membrane is capable of long-term potentiation, or LTP, a hallmark of biological learning and memory. Their work is the first evidence that a cell membrane alone — without proteins or other biomolecules embedded within it — is capable of LTP that persists for many hours.

"We decided to revisit a system previously studied by Pat Collier and co-workers," at ORNL's Center for Nanophase Materials Sciences, said John Katsaras, a biophysicist in ORNL's Neutron Sciences Directorate, "but this time with an entirely different electrical stimulation protocol that we termed 'training.'" This led to data that are practically indistinguishable from the LTP signal observed in the human brain.

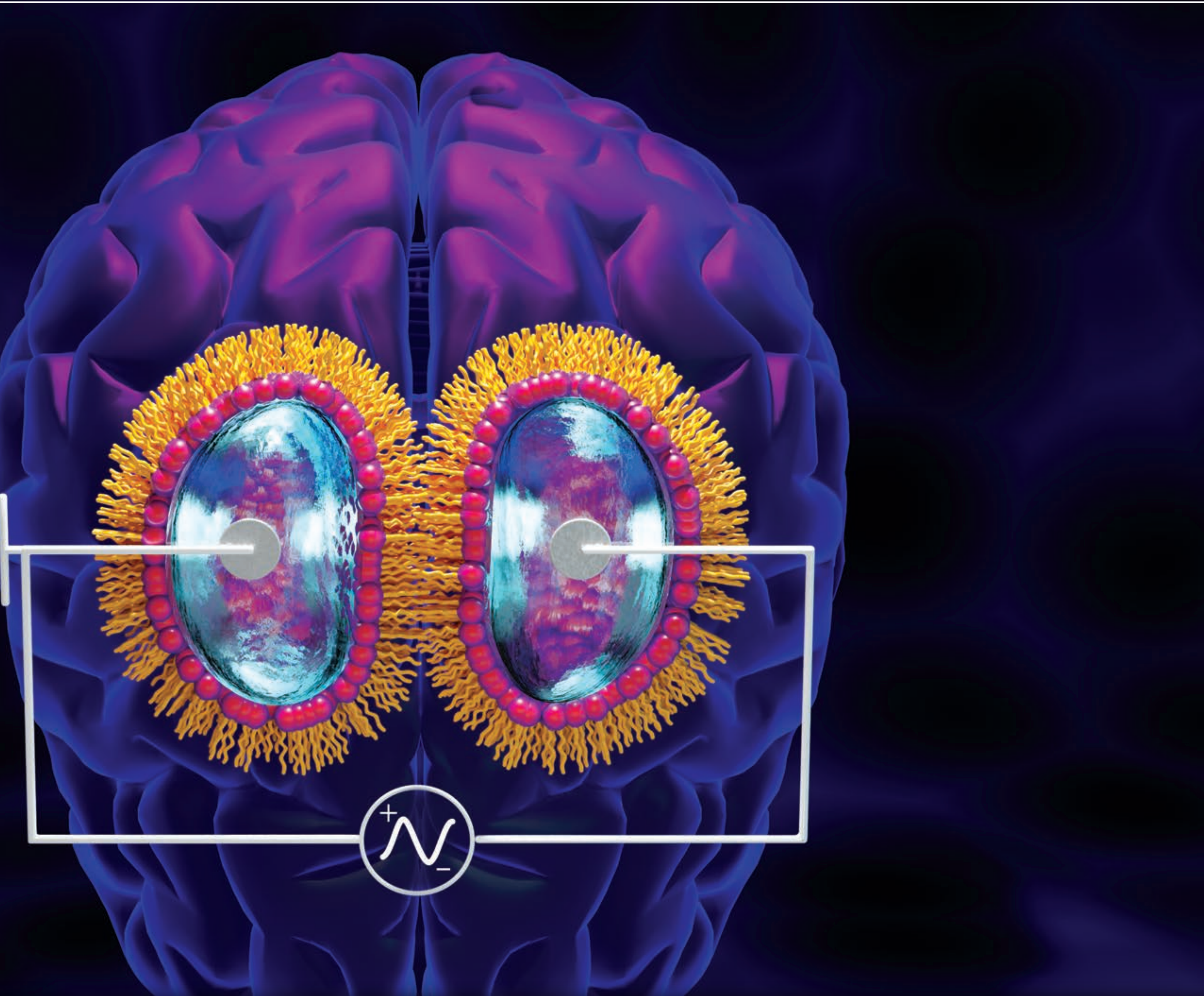
> *Memory and logic in the brain are intertwined. But in modern computers, these functions happen in different locations — an obstacle to performance that the brain does not have.*
>
> — ORNL computational scientist **Pat Collier**

Encoding memory in nanoscale systems has the potential to inform the development of next-generation computing materials and architectures that seek to match the efficiency and flexibility of human cognition — known as neuromorphic computing. Brain-like computation could both advance the performance of artificial intelligence and dramatically alter the energy efficiency and computing capabilities of next-generation devices.

"Memory and logic in the brain are intertwined," said Collier, a staff research scientist at CNMS, where the research was performed. "But in modern computers, these functions happen in different locations — an obstacle to performance that the brain does not have."

Even today's supercomputers have separate locations for processing and memory, requiring them to expend energy and time ferrying information back

A pure lipid membrane formed using lipid-coated water droplets exhibits long-term potentiation, or LTP, which is associated with learning and memory, thus emulating the hippocampal LTP observed in the brains of mammals and birds. Image credit: Jill Hemman, ORNL



and forth. By merging these functions, neuromorphic computers could gain the speed and efficiency needed to keep pace with the exponential growth in data sets that are becoming more complex as the Internet of Things and the interconnectivity of devices become commonplace in homes and workspaces. It would also greatly advance edge computing — the ability of a device to perform its own logic at the site of data collection, without having to send information to a central location.

The nanoscale systems used in this study create an artificial membrane by bringing together two micron-sized lipid-coated water droplets within an oil suspension. At the interface between the two droplets, the lipid bilayer mimics cell membranes at the junctions between nerve cells in the human brain.

Previous ORNL research showed that this biomembrane system is capable of storing an electric charge, but only for short periods of time. In the new study, the presence of LTP means that there are new avenues for how this soft material system could be used in neuromorphic devices or how it can serve as a model for the construction of solid-state devices with similar features.

"Now that we've begun to define the electrical protocols to induce LTP in lipid bilayer membranes, we are preparing to make two-terminal crossbar architectures in which multiple nanoscale membranes interact, allowing for active logic to be performed, not just passive storage," Collier said. "Right now, we're using single systems; going forward, we need to learn how to wire them together."

Anode material

paves the way for fast battery charging

by Ashley Huff
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Researchers at ORNL and the University of Tennessee, Knoxville, discovered a key anode material needed for fast-charging lithium-ion batteries. The commercially relevant approach opens a potential pathway to improve charging speeds for electric vehicles.

Lithium-ion batteries, or LIBs, can store more energy, charge faster and last longer than traditional lead-acid batteries; as a result, they play an essential role in the nation's clean energy portfolio. However, the technology is still developing, and fundamental advances are needed to improve the cost, range and charge time of electric-vehicle batteries.

"Overcoming these challenges will require advances in materials that are more efficient and synthesis methods that are scalable to industry," said ORNL Corporate Fellow Sheng Dai.

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> *Our approach focuses on nongraphite materials. But these also have limitations. Some of the most promising materials — niobium-based oxides — have complicated synthesis methods that are not well suited to industry.*
>
> — ORNL researcher **Runming Tao**

The ORNL and UT team demonstrated a novel compound of molybdenum-tungsten-niobate, or MWNO, with fast rechargeability and high efficiency that could replace graphite in commercial batteries.

For decades, graphite has been the best material for making LIB anodes. In basic battery design, two solid electrodes — a positive cathode and a negative anode — are connected by an electrolyte solution and a separator. In LIBs, lithium ions in the electrolyte move back and forth between the cathode and anode to store and release energy that powers devices.

One challenge for graphite anodes is that the electrolyte decomposes and forms a buildup on the anode surface during charging. This buildup slows the movement of lithium ions and can limit battery stability and performance.

"Because of this sluggish lithium-ion movement, graphite anodes are seen as a roadblock to extreme fast charging. We are looking for new low-cost materials that can outperform graphite," said ORNL's Runming Tao. DOE's extreme fast-charging goal for electric vehicles is 15 minutes, which would be competitive with the refuel times of gas-powered vehicles. The 15-minute milestone has not been met with graphite.

"Our approach focuses on nongraphite materials," Tao said, "but these also have limitations. Some of the most promising materials — niobium-based oxides — have complicated synthesis methods that are not well suited to industry."

ORNL postdoctoral researcher Runming Tao, pictured with a coin cell battery, led an effort to discover new anode materials for fast-charging lithium-ion batteries. Image credit: Genevieve Martin, ORNL

Conventional synthesis of niobium oxides such as MWNO is an energy-intensive process over open flame that also generates toxic waste. A practical alternative could make MWNO materials serious candidates for use in advanced batteries.

The researchers turned to the well-established sol-gel process, known for its safety and simplicity. Unlike conventional high-temperature synthesis, the sol-gel process is a low-temperature chemical method for converting a liquid solution into a solid or gel material and is commonly used to make glasses and ceramics.

The team transformed a mixture of ionic liquid and metal salts into a porous gel that was treated with heat to enhance the material's final properties. The low-energy strategy also enables the ionic liquid solvent used as a template for MWNO to be recovered and recycled.

"This material operates at a higher voltage than graphite and is not prone to forming what is called a 'passivation solid electrolyte layer' that slows down the lithium-ion movement during charging," Tao said. "Its exceptional capacity and fast-charging rate, combined with a scalable synthesis method, make it an attractive candidate for future battery materials."

The key to the material's success is a nanoporous structure that provides enhanced electrical conductivity. The result offers less resistance to the movement of lithium ions and electrons, thus enabling fast recharging.

"The study achieves a scalable synthesis method for a competitive MWNO material, as well as providing fundamental insights on future design of electrode materials for a variety of energy storage devices," Dai said.

Adsorbent material

filters toxic chromium, arsenic from water supplies

by Ashley Huff
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Chromium and arsenic are two of the most dangerous pollutants found in drinking water.

Both are toxic and can cause adverse health effects, including cancer. Even low levels pose significant risks to living organisms because the substances bioaccumulate, or build up with each exposure, and can gradually reach harmful amounts.

These elements occur naturally, but their presence in the environment has increased over time as byproducts of mining and manufacturing. Releases impact air, soil and water, but drinking water is the most common route of exposure.

Organic chemists at ORNL are tackling the challenge with a unique material designed to target chromium and arsenic for simultaneous removal.

"It is rare for an adsorbent to capture two pollutants simultaneously and to work quickly and efficiently in realistic scenarios to address the broad range of water conditions worldwide," said ORNL's Santa Jansone-Popova.

Jansone-Popova is part of an ORNL group specializing in the study of adsorbents, materials that target specific elements and bind them to a surface. Adsorbents are widely used to recover precious metals and remove pollutants from the environment.

"They are one of the most promising water treatment options because they are affordable, easily deployed and can work quickly to filter water supplies, but they need to be tailored for practical use in cleanup scenarios," Jansone-Popova said. "The challenge is to design materials that can effectively isolate trace amounts of harmful elements that are very similar to the bulk chemical species found in water."

Jansone-Popova and colleague Ping Li, who is now at Elementis Global, discovered an adsorbent that effectively removes chromium and arsenic in real conditions where water resources contain many chemically similar elements. The fundamental advance works by creating synergy, meaning the more chromium the material grabs, the more arsenic it can also remove.

In water, these heavy metals dissolve to form chromate and arsenate oxoanions — salts that are chemically similar to beneficial minerals that are naturally present in water. These salts include phosphate, sulfate, nitrate and bicarbonate. Chromate and arsenate are highly mobile in water and can have far-reaching impacts. They do not degrade and are permanent in the environment without intervention. Targeted approaches are needed to separate these metals from harmless mineral salts that are vital to the ecosystem.

In adsorbent design, selectivity is key. Because a material's surface offers limited

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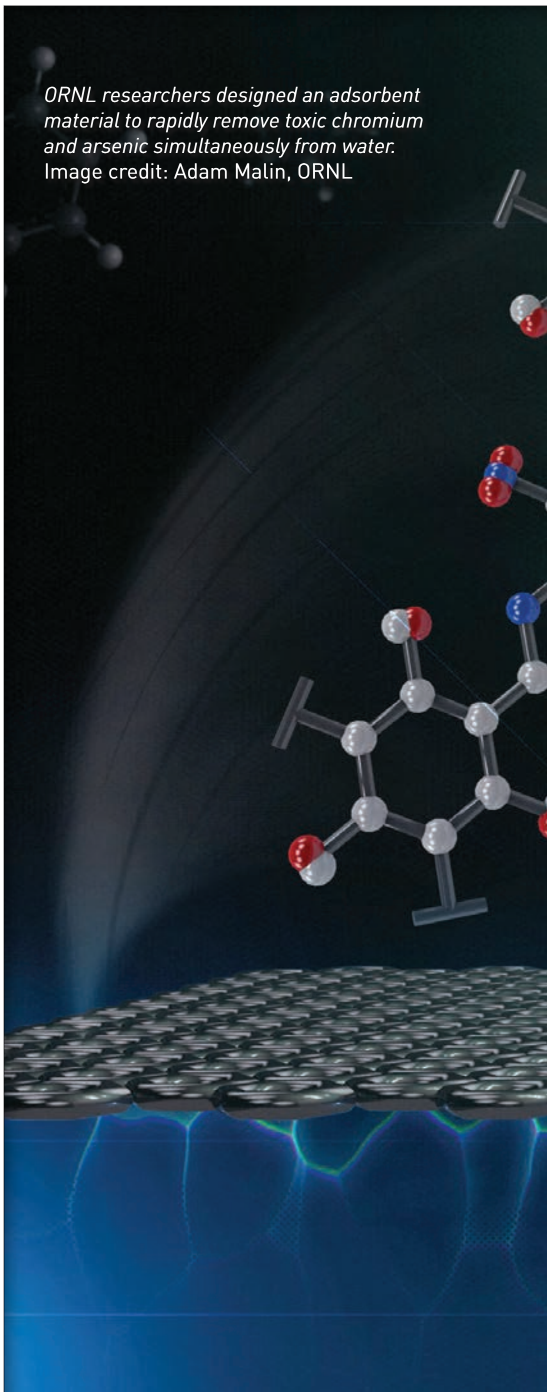
Fundamental discoveries like these can help us reduce toxic pollutants in the environment and meet regulatory goals for clean water.

— ORNL researcher **Santa Jansone-Popova**



ORNL researchers designed an adsorbent material to rapidly remove toxic chromium and arsenic simultaneously from water. Image credit: Adam Malin, ORNL real estate, the goal is to grab only the targeted elements and capture as much as possible before the adsorbent fills up and needs to be replaced or recycled. Poorly selective materials lack the precision to single out targets in mixed environments such as water, where similar elements compete for space.

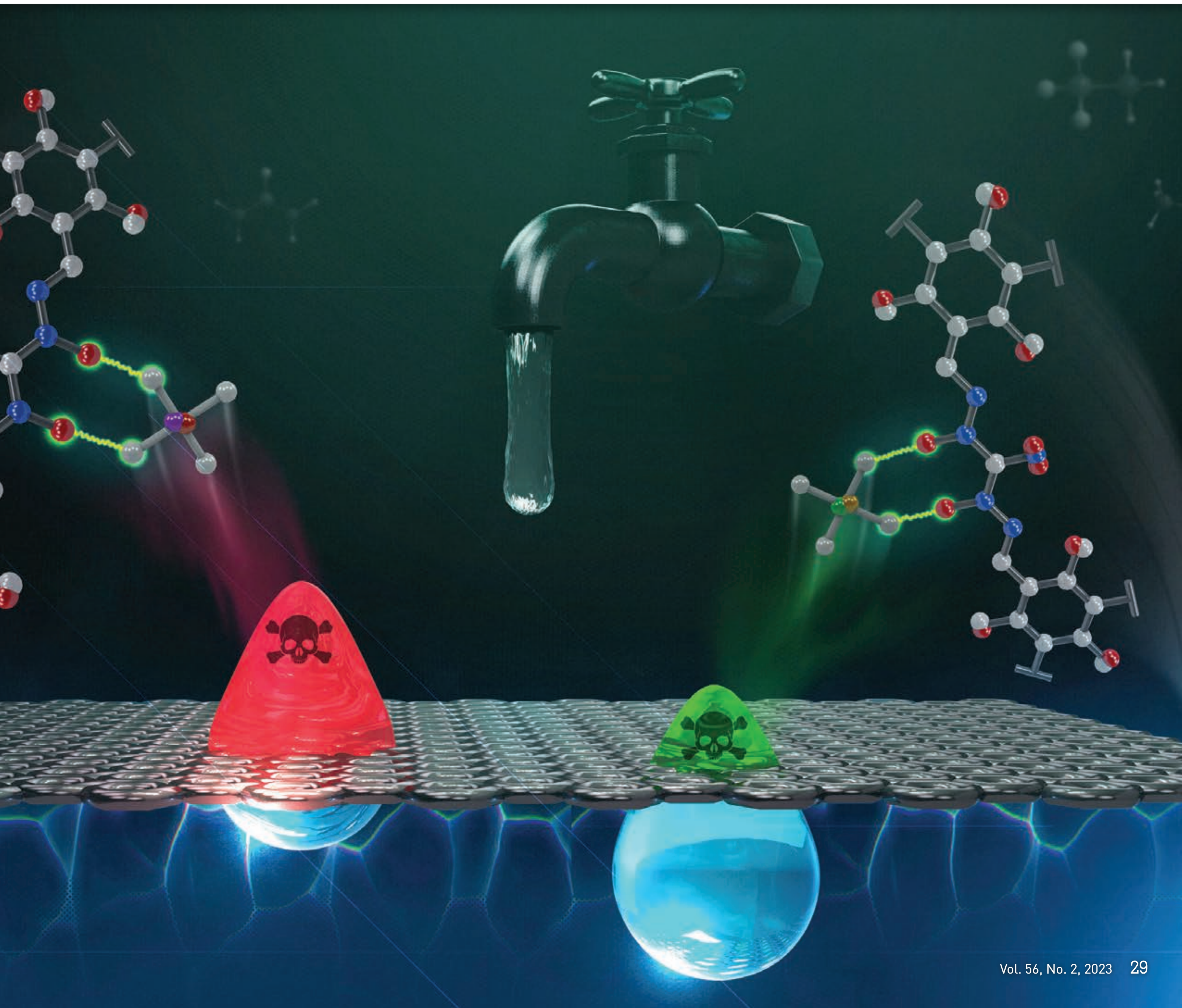
The team drew from a previous ORNL discovery on chromium capture to create a platform for new chemistry that would also bind arsenic.

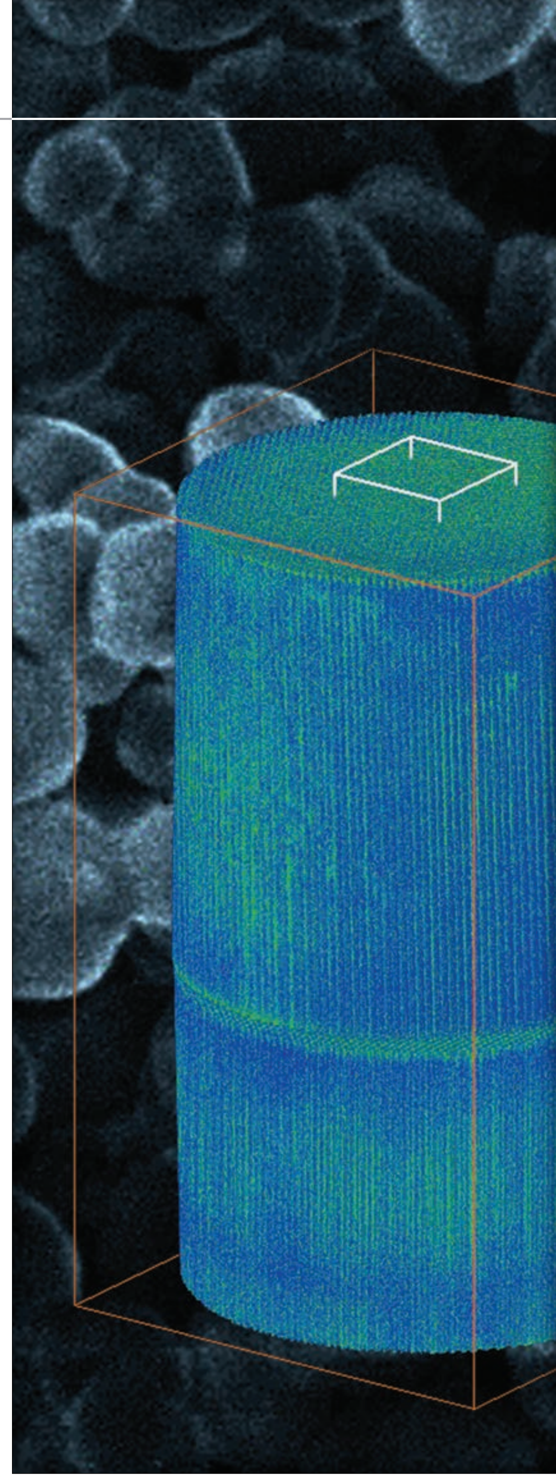
The starting material effectively trapped chromium in its most toxic form — known as hexavalent chromium, or chromium-6 — but was not selective for arsenic. Researchers modified the material's structure to convert captured chromium-6 into a less toxic state, chromium-3. Chromium-3 also has the benefit of providing an anchor point to bind arsenate.

The new structure enables a chemical reaction that forms stable chromate-arsenate clusters that are strongly bonded to the surface. The result effectively traps the toxins permanently because they will not wash off or detach from the filter material without intentional removal by chemical processing.

The team has patented the structure and is working with collaborators to expand the approach to other environmental pollutants.

"Fundamental discoveries like these can help us reduce toxic pollutants in the environment and meet regulatory goals for clean water," Jansone-Popova said.





Add-on device

makes home furnaces cleaner

by Paul Boisvert
boisvertpl@ornl.gov

Natural gas furnaces not only heat your home, they also produce a lot of pollution.

Even modern high-efficiency condensing furnaces produce significant amounts of corrosive acidic condensation and unhealthy levels of nitrogen oxides, carbon monoxide, hydrocarbons and methane. These emissions are typically vented into the atmosphere and end up polluting our soil, water and air.

Now, ORNL scientists have developed an affordable add-on technology that removes more than 99.9 percent of acidic gases and other emissions to produce an ultraclean natural gas furnace. This acidic gas reduction, or AGR, technology can also be added to other natural gas-driven equipment such as water heaters, commercial boilers and industrial furnaces.

"Just as catalytic converters help reduce emissions from billions of vehicles worldwide, the new AGR technology can virtually eliminate problematic greenhouse gases and acidic condensation produced by today's new and existing residential gas furnaces," said Zhiming Gao, staff researcher with ORNL's Energy Science and Technology Directorate. "An eco-friendly condensate also eliminates the need to use corrosion-resistant stainless steel materials for furnace heat exchangers, which reduces manufacturing costs."

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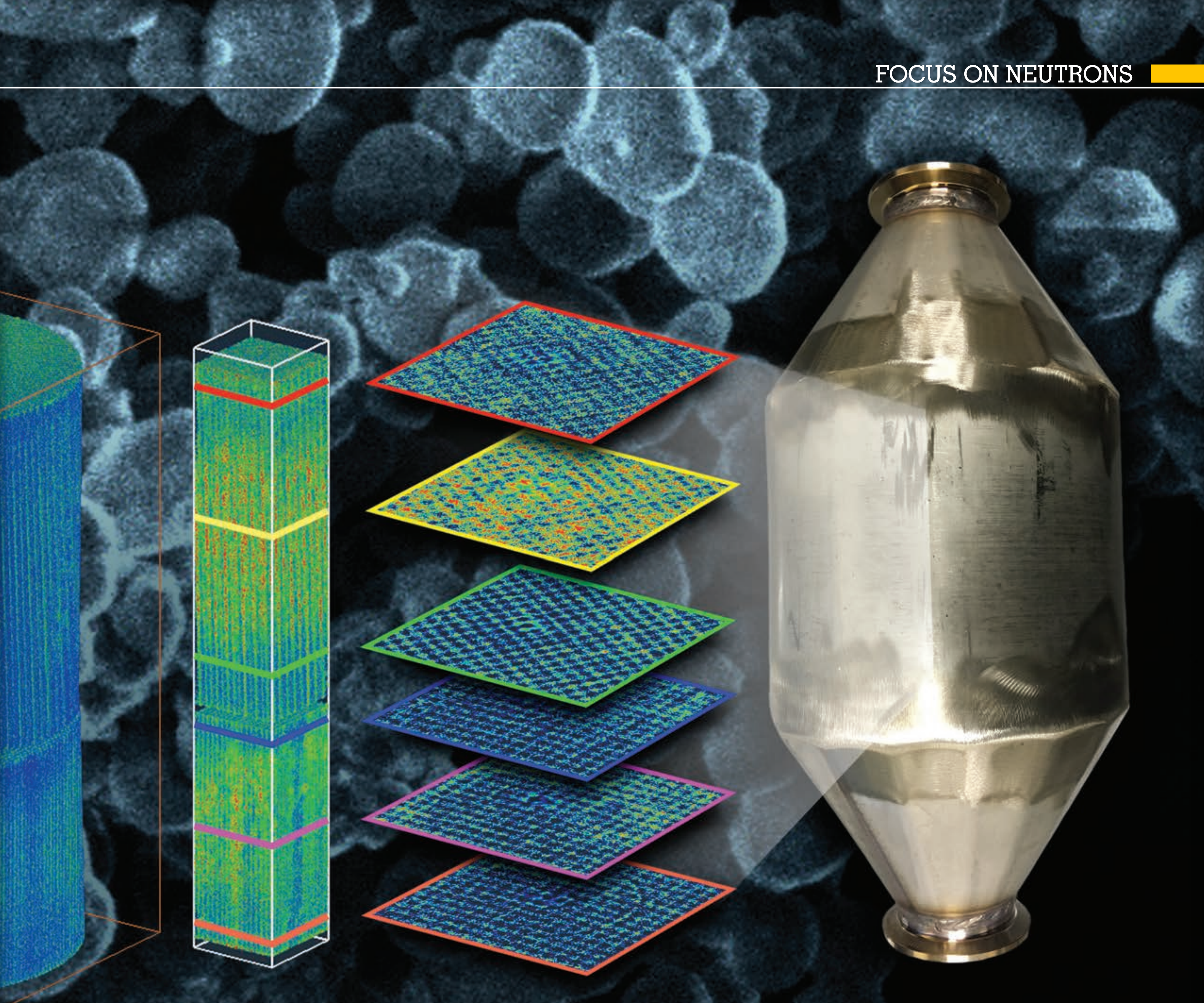
— ORNL researcher **Zhiming Gao**

To demonstrate the effectiveness of AGR in a furnace, the researchers fabricated an AGR catalyst, enclosed it in a metal housing and installed the device on a standard commercially available high-efficiency condensing furnace. Results after a 400-hour reliability and durability test showed the AGR almost completely removed harmful emissions from the flue gas and produced a nonacidic condensate with a neutral pH level.

To examine the furnace's internal condition and soot distribution after the test without damaging the device's gas flow-through channels, the scientists used neutron computed tomography at ORNL's High Flux Isotope Reactor, or HFIR. Unlike X-rays, neutrons can penetrate the metal housing to record images that are then used to produce 2D and 3D representations of the used device.

"Such insights will enable improved AGR device designs for a more uniform and self-cleaning gas flow pattern," Gao said. "This will also help alleviate excessive soot



ORNL's award-winning ultraclean high-efficiency condensing natural gas furnace features an affordable add-on technology that can remove more than 99.9 percent of acidic gases and other emissions. Image credit: Jill Hemman, ORNL

accumulation to enhance AGR-enabled furnace performance."

Soot particles, which typically form because of the incomplete combustion of hydrocarbons, contain substantial hydrogen. Neutrons are especially good at detecting and mapping hydrogen and other light elements.

"Neutron imaging and mapping after the AGR test provided details about how the flue gas flowed through the AGR, which revealed the heavy accumulation of soot particles in the middle of the catalyst," said Yuxuan Zhang, a neutron instrument scientist at HFIR.

AGR technology would allow furnace manufacturers to use materials that are more affordable than the stainless steels used in most heat exchangers. This increased affordability could allow furnace manufacturers to sell more high-efficiency furnaces that meet California's proposed new standards for residential and commercial furnace emissions.

"Currently, AGR-enabled furnaces would require offline regeneration of the device about once every three years under normal use conditions," Gao said. "The AGR unit could be removed by a homeowner or technician and carried to a regeneration and recycling location. This would be similar to how consumers bring their empty natural gas tanks for their outdoor grills to a dealer to exchange them for full tanks."

In 2022, the ORNL AGR technology received a coveted R&D 100 award and was selected for targeted investment through ORNL's Technology Innovation Program.

Location intelligence

shines a light on disinformation

by Sumner Brown Gibbs
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Using disinformation to create political instability and battlefield confusion dates back millennia.

However, today's disinformation actors use social media to amplify disinformation that users knowingly — or, more often, unknowingly — perpetuate. Such disinformation spreads quickly, threatening public health and safety. Indeed, the COVID-19 pandemic and recent global elections have given the world a front-row seat to this form of modern warfare.

A group at ORNL now studies such threats thanks to location intelligence, or research that uses open data to understand places, as well as the factors that influence human activity in those places. In the past, location intelligence has informed emergency response, urban planning, transportation planning, energy conservation and policy decisions. Now, ORNL uses location intelligence to identify disinformation, or shared information that is intentionally misleading, and its impacts.

"Up until now, we knew disinformation campaigns existed online, but we did not know how the disinformation flowed," said Gautam Thakur, leader of ORNL's Location Intelligence Group. "By bridging a gap between the virtual world and the physical world, we can now help provide insights that agencies and organizations can use to counteract such threats."

Today's disinformation campaigns spread fast and deep as disinformation actors carefully craft their messages to target specific audiences. To spread disinformation, these actors often use bots, or computer algorithms that emulate human behavior online. Only a few narratives need to catch on to create vulnerability, build cohesion among extremist groups or erode civil trust.

Some of the group's latest work involves understanding how to measure the intent of social media users based on tweets sent during the COVID-19 pandemic.

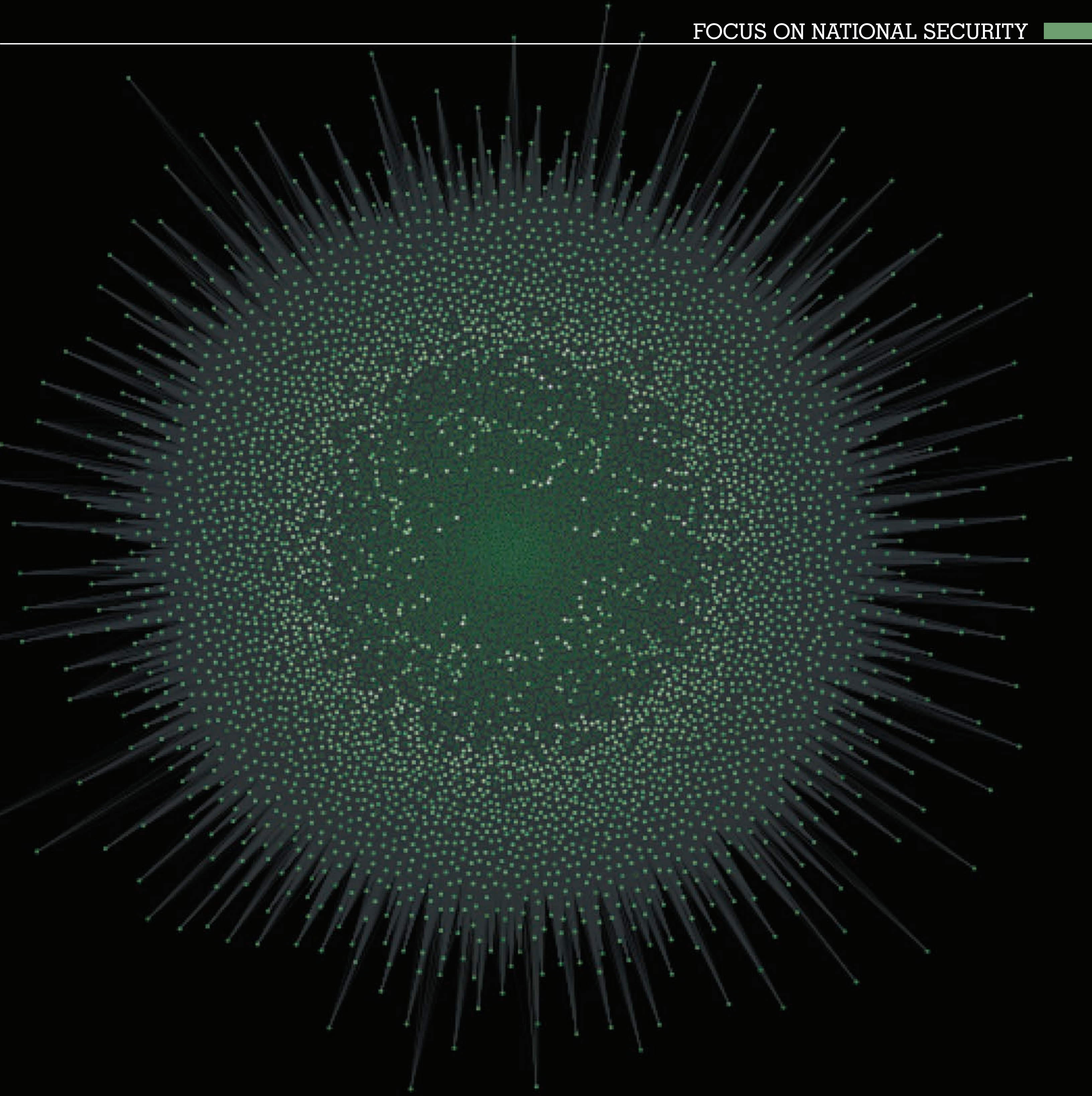
"We discovered we needed an automated method to quantify the intent of all social media users to help keep the public safe from disinformation actors," said Chathika Gunaratne, a postdoctoral researcher in ORNL's Computing and Computational Sciences Directorate.

With help from computational data engineer Varisara Tansakul and data science researcher Debraj De, the multidisciplinary team tested a new approach on 4.7 million COVID-19–related tweets from more than 14,000 users. The team combined the results of this study with its other study results on intent and disinformation. Because of these efforts, the team can now correlate breaking news notifications with disinformation actors' online responses, incorporating information such as the unique spatial patterns of information spread and the methods used by social media users to intensify this spread.

Thakur began collecting data on human activities when he came to ORNL in 2013, but he soon realized the lab needed the ability to characterize — in real time — the human behaviors that were driving the data. Then, in 2015, ORNL released PlanetSense, a digital platform used to analyze online crowd-sourced data in real time.

PlanetSense enables researchers to study human activity through the lenses of economy, culture and social ties and to illustrate how and why things happen in different places. PlanetSense now under-

> *We discovered we needed an automated method to quantify the intent of all social media users to help keep the public safe from disinformation actors.*
>
> — ORNL researcher **Chathika Gunaratne**



Each dot represents a Twitter user discussing COVID-19 between April 16 and April 22, 2021. The closer the dots are to the center, the greater the influence. The brighter the color, the stronger the intent. Image credit: ORNL

pins the development of other digital tools ORNL uses in human dynamics research.

"While we build computing systems that capture data from points of interest across the entire planet, it is really understanding the cultural and social ties that allows us to better understand human activities," Thakur said. "In order to help agencies and organizations respond to certain events, we need to be able to make sense of the data, which means we must be ready to narrate certain activities as they are happening. This requires a very interdisciplinary approach, which is possible at ORNL given our breadth of foundational sciences."

For more information: https://www.osti.gov/biblio/1891407

Scientific computing at ORNL

SPEC

ORNL's first computer is a matrix multiplier that supports the lab's nuclear-powered-aircraft research.

1947

iPSC

5.12 gigaflops

This Intel Personal SuperComputer is ORNL's first system to top a gigaflop, or a billion calculations per second.

1988

Eagle

When this IBM RS/6000 SP system is upgraded in 2000, it will become the first DOE Office of Science computer to top a teraflop, or a trillion calculations per second.

1998

1950 1960 1970 1980 1990

1953

ORACLE

100 kiloflops

The Oak Ridge Automatic Computer and Logical Engine has the fastest speed and largest data storage capacity of any computer in the world.

1995

Intel Paragon

150 gigaflops

This Intel Paragon XP/S 150 system is the world's fastest.

2004

Phoenix

3 teraflops

The world's largest Cray X1, Phoenix helps explain the forces that influence electron flow in high-temperature superconductors.

ORNL has pioneered scientific computing for more than seven decades, dating back to the creation of the Mathematics and Computing Section in 1947. Here are some key milestones in the lab's computing history.

Jaguar (XT3)

26 teraflops

The first iteration of Jaguar will be upgraded to 54 teraflops.

2005

Titan

27 petaflops

This Cray XK7 will debut at No. 1 on the Top500 List and is the first major supercomputer with a hybrid architecture of central processing units and graphics processing units.

2012

Frontier

1.7 exaflops

This HPE-Cray EX system — currently No. 1 on the Top500 List — is the world's first supercomputer to top an exaflop, or a quintillion calculations per second.

2022

2000 2010 2020

2008

Jaguar (XT5)

1.6 petaflops

This iteration of Jaguar is ORNL's first system to top a petaflop, or a quadrillion calculations a second. It will spend a year at No. 1 on the Top500 List of the world's most powerful supercomputers.

2018

Summit

200 petaflops

This IBM AC922 will spend two years at No. 1 on the Top500 List.

Future

Scientific computing will increasingly turn to machine learning, artificial intelligence and hybrid systems that incorporate quantum computing.

Image credit: Brett Hopwood, ORNL

Tiny, revved-up microbe

tackles big plastics challenge

by Stephanie Seay
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To resolve the challenge of difficult-to-recycle plastic waste, ORNL scientists used their bioengineering expertise to create a new ally: a specially designed microorganism with an appetite for converting mixed plastic into new, sustainable products.

Only about 5 percent of plastic is recycled, mostly because products vary in their chemical makeup, and separating and treating them is difficult and costly.

Researchers seeking biobased solutions came up with a two-step chemical and biological process to break down and upcycle mixed plastics into valuable new bioproducts, skipping the sorting. The work was performed as part of a Department of Energy consortium called BOTTLE, for Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment.

"Plastics are major environmental pollutants and are largely made using fossil carbon," said ORNL genetic engineer Adam Guss. "This research sits at that intersection of breaking down today's plastic waste and converting it into building blocks for the next generation of plastics that are both recyclable by design and biodegradable."

The first step relies on oxygen and catalysts to break down large polymer molecules into their smaller chemical building blocks. The process was applied to a mixture of three common plastics: polystyrene, used in disposable coffee cups; polyethylene terephthalate, or PET, used in single-use beverage bottles, polyester clothing and carpets; and high-density polyethylene, used in many common consumer plastics such as milk jugs.

The oxidation process breaks down these plastics into a complex mixture of chemical compounds — including benzoic acid, terephthalic acid and dicarboxylic acids — that would require advanced and costly separations to yield pure products. That is where microbes come into play.

BOTTLE researchers engineered a soil microbe, *Pseudomonas putida*, to biologically convert the mixture of small molecules into single products: either polyhydroxyalkanoates, which are an emerging form of biodegradable bioplastics, or beta-ketoadipate, which can be used to make new nylon materials.

The experiment built on a process developed by Guss and colleagues at ORNL and the National Renewable Energy Laboratory to engineer the bacterium with desired traits from other organisms. The process converted deconstructed

ORNL genetic engineer Adam Guss examines a petri dish of microbes at ORNL. Image credit: Carlos Jones, ORNL

Adam Guss in a synthetic biology lab at ORNL. Image credit: Carlos Jones, ORNL

PET into building blocks for a superior nylon product that is more water- and heat-resistant than other such products, making it ideal for applications such as automotive parts.

> *Plastics are major environmental pollutants and are largely made using fossil carbon. This research sits at that intersection of breaking down today's plastic waste and converting it into building blocks for the next generation of plastics that are both recyclable by design and biodegradable.*
>
> — ORNL genetic engineer **Adam Guss**

"We took a combinatorial approach to pathway assembly, basically finding the best combination of genes from different organisms that allowed us to get robust utilization of PET in *Pseudomonas putida*," Guss said. ORNL specializes in modifying microbes to add traits useful for biotechnology, including applications for the production of biofuels and industrial chemicals.

Guss and colleagues have spent years perfecting *P. putida* to convert lignin, a plant biopolymer derived from bioenergy crops, into advanced bioproducts as part of DOE's Center for Bioenergy Innovation at ORNL. He conducts similar work for the DOE Agile BioFoundry, which brings together national labs and industry to develop biomanufacturing technologies. In 2020, Guss led a team that announced it had engineered the microbe to simultaneously digest five of the most abundant compounds of lignocellulosic biomass, the material obtained from breaking down plants to make naturally derived fuels and other products.

In the next steps for BOTTLE, "we're continuing to expand the range of molecules that *P. putida* can eat as we work to break down more types of plastics with additional additives," Guss said.

Funding for the research was provided by DOE's Advanced Manufacturing Office and Bioenergy Technologies Office through the BOTTLE consortium.

Neutrons reveal

how the spider lily preys on cancer cells

by Sumner Brown Gibbs
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A scientific instrument at ORNL could help create a noninvasive cancer treatment from a common tropical plant.

Pancratistatin is a chemical compound found in the spider lily, a native Hawaiian flower. Unlike traditional treatments, it kills cancer cells while keeping healthy cells intact.

Until recently, pancratistatin's workings mystified scientists, clouding hope for potential new treatments. But after conducting neutron experiments at ORNL, students from the University of Windsor have gained fundamental insights into the mechanics of pancratistatin that could open new doors to much-improved cancer treatments.

"By experimenting with cellular extracts here at the lab, we're building on previous work to get a more detailed picture for pancratistatin," said Stuart Castillo, the UWindsor doctoral candidate leading the study. "Our hope is to create a new path for treating cancer that doesn't damage healthy cells."

ORNL's Spallation Neutron Source provides one of only a handful of neutron instruments in the world capable of making the measurements the study needed. The Neutron Spin Echo instrument allowed the students to simultaneously measure cellular dynamics in angstroms and microseconds. One angstrom equals one ten-billionth of a meter. One microsecond equals one millionth of a second.

Cancerous tumors begin with cells that reproduce when they should not. This process starts in mitochondria, the parts of a cell that produce energy. In theory, cancer cells get an influx of cholesterol that stiffens mitochondrial membranes, stopping their communication with other parts of the cell. Then, the mitochondria go rogue, causing cells to overmultiply.

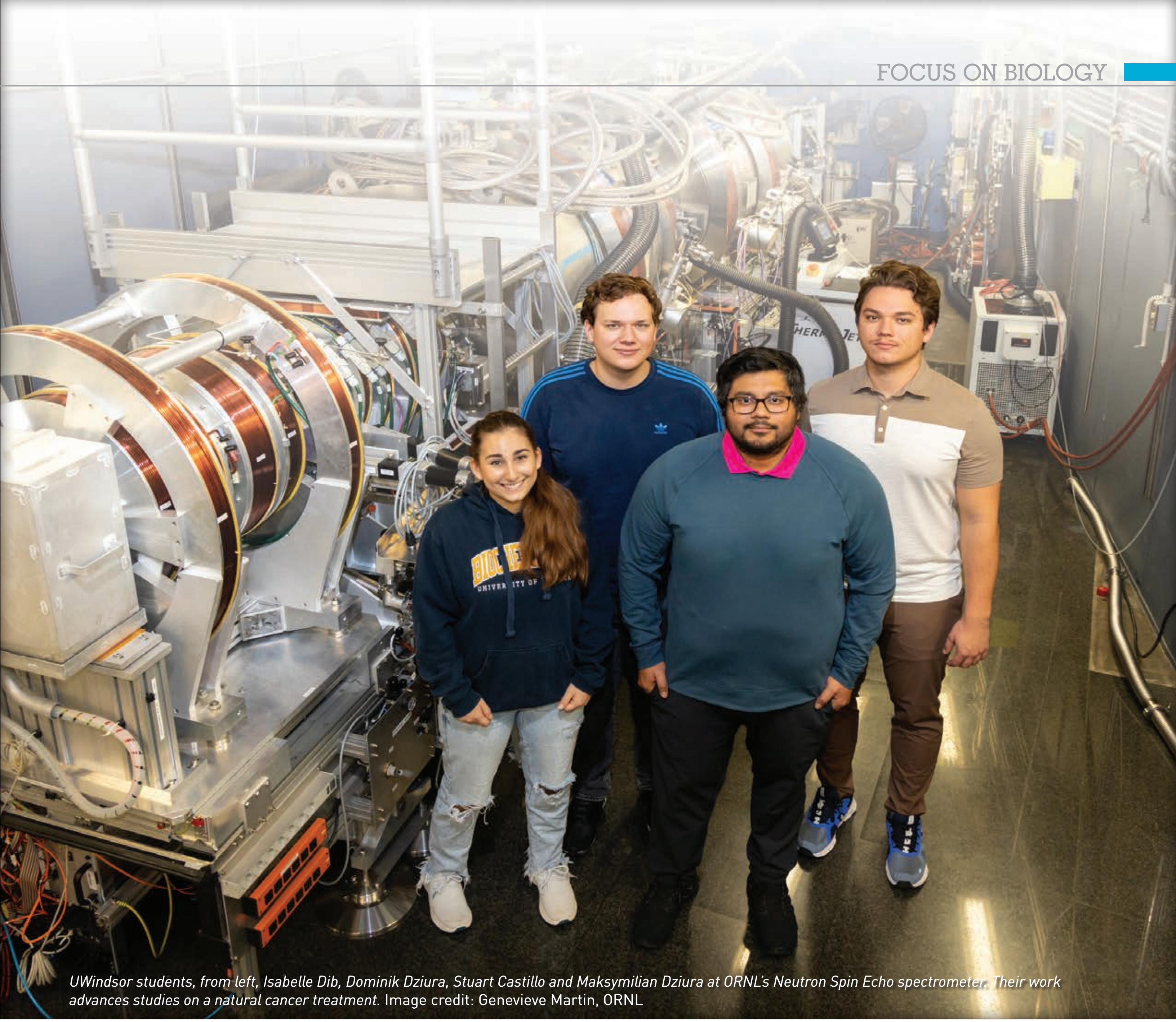
By experimenting with cellular extracts here at the lab, we're building on previous work to get a more detailed picture for pancratistatin. Our hope is to create a new path for treating cancer that doesn't damage healthy cells.

— UWindsor doctoral candidate **Stuart Castillo**

One step back, one leap forward

Decades ago, scientists used living cells to discover pancratistatin's effect on cancer. In these early experiments, pancratistatin successfully triggered apoptosis, or cell death, in cancerous testicular, breast, liver, pancreatic and nerve cells. Since then, research has been confined to experiments on synthetic membranes until more could be understood about this natural remedy. Experimenting with synthetic material allows researchers to build their understanding of specific changes without the variables that come with living systems.

"Something we say about working with synthetic membranes is that it's never 100 percent representative of a cell and never will be," said UWindsor graduate researcher Maksymilian Dziura. "We want to use living cells to understand cells, but getting there isn't easy. We need to fully understand the picture before we can slowly transition into using more realistic systems."



UWindsor students, from left, Isabelle Dib, Dominik Dziura, Stuart Castillo and Maksymilian Dziura at ORNL's Neutron Spin Echo spectrometer. Their work advances studies on a natural cancer treatment. Image credit: Genevieve Martin, ORNL

Neutrons are particularly well-suited for investigating biological membranes because neutrons can pass through delicate biological materials without damaging them. Before coming to ORNL, the students showed that pancratistatin stiffened synthetic mitochondrial membranes in a way that triggered apoptosis, providing the basis for working with cells.

The students used SNS's Neutron Spin Echo spectrometer to compare how pancratistatin affects the inner and outer layers of the mitochondria's membranes in cancerous and noncancerous cells.

"We're looking specifically at how stiff the membrane is, how thick it is and how those molecules behave next to each other," said UWindsor graduate researcher Dominik Dziura. "The thought is that a healthy membrane will be flexible and move like it's supposed to, binding to other receptors and membranes and allowing communication between cells, unlike the cancerous membranes."

"There's so much we don't know about cancer," said UWindsor graduate researcher Isabelle Dib. "And we haven't really looked at the differences between cancerous and noncancerous cellular membranes. This is a new approach."

The team used labs at ORNL's Shull Wollan Center and Center for Nanophase Materials Sciences to develop and prepare their samples. The proximity of these resources enabled the team to do research in a few short weeks that otherwise could have taken them months or longer.

"The setup we have here, with SNS, the Shull Wollan Center and CNMS, it's perfect for us to conduct our experiments and analyze our data," said Castillo. "It's the whole package."

East Tennessee looks to bolster nuclear workforce

by David Keim
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The East Tennessee Economic Council brought together leaders from industry, government contractors, universities and economic development organizations this summer to begin defining needs for the region's nuclear workforce.

At ORNL's request, ETEC convened two meetings in June through its Nuclear Working Group. Interim Laboratory Director Jeff Smith said the goal was to be sure ORNL is focusing on a topic that can most help the community.

"Our region has an opportunity to distinguish itself from others due to the unique variety of resources already in place," Smith said. Those resources go well beyond the expertise found at ORNL to include the uranium expertise of the nearby Y-12 National Security Complex, the strength of the University of Tennessee's nuclear engineering program, and the presence of more than 200 companies associated with the nuclear industry.

"A skilled workforce is foundational to realizing our region's potential, and companies need to know that we're serious about addressing workforce gaps," Smith said.

The East Tennessee effort complements Tennessee Gov. Bill Lee's appointment of a Nuclear Energy Advisory Council, which includes Smith and ETEC President Tracy Boatner among area representatives.

The state also set up a $50 million Nuclear Fund to "establish a nuclear development and manufacturing ecosystem built for the future of Tennessee by providing grants and assistance to support nuclear power-related businesses that choose to relocate or grow in the state."

The Nuclear Working Group's discussions focused on workforce needs across six nuclear sectors: the front and back ends of the fuel cycle, from fuel fabrication to waste disposal; power plants; medical isotopes; nuclear security; and fusion energy.

ETEC President Tracy Boatner addresses the Nuclear Opportunities Workshop. Image credit: East Tennessee Economic Council

During the Nuclear Opportunities Workshop in August, UT-Battelle Interim President and CEO Jeff Smith, left, presented Roane State President Chris Whaley with a $100,000 check to help launch a Nuclear Technology Program at the college. Image credit: David Keim, ORNL

"A big part of what sets Tennessee apart is the variety of nuclear-related work taking place here," Boatner said. "We have leaders in areas from research to energy production to radioisotopes. We have public and private growth in fusion energy. And of course we have some of the leading expertise in nuclear security in the world. There is no better place for nuclear industries across the spectrum."

In ETEC's discussions, common job types emerged across sectors, including nuclear safety, radiation control, project controls and skilled craft. The discussions emphasized the need to maintain growth in the pipeline of scientists, too, and participants proposed ideas such as partnering colleges and universities with regulatory bodies for specialized certifications to equip graduates for nuclear jobs.

Altogether, brainstorming highlighted dozens of workforce needs as well as potential partners for addressing those needs, ranging from DOE and its contractors to colleges, trade schools, universities, the Tennessee Valley Authority and area companies.

At ETEC's Nuclear Opportunities Workshop in August, Smith shared an illustration headlined "Nuclear is Here" that captured the results of the working group's discussions. He encouraged business and community leaders to consider how they could help to build the nuclear workforce.

To demonstrate the commitment of ORNL contractor UT-Battelle, Smith announced a $100,000 contribution for a nuclear technology program at nearby Roane State Community College. The funds will purchase instruments, nuclear sources and tools for a nuclear measurements lab serving an estimated 10 to 20 students beginning in the fall of 2024.

Smith urged each NOW attendee to identify and address a need on the "Nuclear is Here" graphic.

"Collectively, we will begin to distinguish this state as a state that is serious about solving the workforce challenge, especially in nuclear," Smith said. "That's going to be really important to the next company that shows up and wants to know whether this is home for them."

He said the contribution doesn't need to be huge.

"If you can just support one intern for a summer, that would be an important contribution. If you can help someone buy a piece of equipment, don't walk away from here feeling you don't have the opportunity to contribute. I think you all do."

3D-printed home

made from biobased materials

by Jennifer Burke
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On the grounds of the University of Maine's Advanced Structures and Composites Center sits the nation's first additively manufactured home made from biobased materials — BioHome 3D.

The 600-square-foot home is a test bed to see how well the materials perform. If environmental analysis, weatherization testing and energy data–gathering prove favorable, then thousands of similar homes may be manufactured, providing an energy-efficient and economical housing alternative in the U.S.

While BioHome is located thousands of miles from ORNL, the foundational research that led to its completion traces back to a bamboo-based 3D-printed pavilion showcased in Miami in 2016.

"We were asked by an architectural firm to print large-scale components from environmentally friendly material for a pavilion for a design exposition," said Soydan Ozcan, an ORNL materials scientist who leads research with UMaine. "We chose bamboo." The result was more than 10,000 pounds of printed material.

"We began compounding bamboo to make pellets, just in small batches at first," he said. "This was also the first time a bioderived or biobased material was used for a large-scale additive manufacturing application."

The bamboo was combined with polyactic acid, or PLA, a bioderived and biodegradable thermoplastic polyester also known as a bioplastic. The mixture contained about 20 percent bamboo and 80 percent PLA, with the printed product containing similar properties as wood, including recyclable characteristics. The formulation worked and produced sturdy parts for the pavilion that could withstand the hot and humid Florida climate as well. It also led the research team to consider additional bioderived materials that could be compounded and printed to make other large-scale components for applications such as boats and houses.

> *We began compounding bamboo to make pellets, just in small batches at first. This was also the first time a bioderived or biobased material was used for a large-scale additive manufacturing application.*
>
> — ORNL materials scientis **Soydan Ozcan**

"We were investigating formulations for different materials, and around that time the University of Maine was also interested in developing bioderived materials,"

The fully furnished, additively manufactured home is serving as a testbed to see how the materials perform over time. ORNL researchers embedded sensors in the home to monitor moisture and simulate conditions as if someone were living there. Image credit: UMaine

BioHome 3D sits on the campus of UMaine's Advanced Structures and Composites Center and is made from bioderived materials developed in collaboration with ORNL researchers. Image credit: UMaine

Ozcan said. "This eventually led to printing a mold for the roof for a yacht in 2019."

Made from wood flour, cellulose nanofibrils and PLA, the yacht top marked the first research collaboration between ORNL and UMaine and led to establishment of the first large-scale biobased additive manufacturing program in the U.S. to connect regional industry and university clusters with national lab resources. The collaboration was formed to find a new use for the forest-derived materials previously needed by paper mills in Maine.

Ozcan said the boat component led naturally to discussion about printing much larger objects. While 3D printing a house of bioderived materials had long been seen as a possibility, the U.S. housing shortage sparked an urgent need to move forward. Current estimates put the national shortage of homes at 5.5 million and counting.

"It's not just the shortage of houses, but skilled labor to build them, too," Ozcan added. "This drives the need for automated and digitized construction and additive manufacturing with new materials."

ORNL worked with UMaine researchers to produce the home from novel biobased materials. It's different from other commercially available 3D-printed houses because it was made using fully biobased feedstock and was 100 percent additively manufactured in modules including the floors, walls and roof. The home was printed at UMaine during a single printing session.

Researchers will collect data on the home to further prove that it's a viable construction alternative. "We have sensors that simulate as if someone is living in the house," Ozcan said. "This will help inform what we design next; we can look at printing multilevel homes and integrate energy-efficient equipment so that the home emits no carbon."

While the research home took several months to produce, the goal is to be able to print one home every two days, ultimately helping to alleviate the housing shortage while increasing affordability.

Researchers explore

hydrogen power for railways

by Jennifer Burke
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ORNL researchers are exploring hydrogen as an alternative train fuel to decarbonize the railway industry.

The North American diesel-powered rail fleet emits nearly 90 billion pounds of carbon dioxide a year, making it a major driver of climate change. And while electrification is an effective decarbonization strategy for some parts of the transportation sector, such as vehicles, it is problematic for railways because of the high cost of building a single coordinated electrified rail system. As the United States shifts away from fossil fuels in an effort to reach net-zero carbon emissions by 2050, hydrogen is being studied as an alternative to diesel.

ORNL scientists, working with rail industry provider Wabtec and Argonne National Laboratory, will develop a hybrid locomotive engine over the next four years that can run on both hydrogen and diesel.

A single-cylinder research engine developed by Wabtec has been installed at DOE's National Transportation Research Center at ORNL. Using one cylinder from a locomotive engine model already in use helps researchers understand the production hardware needed for retrofitting.

> *We are excited to be a part of this collaboration because it addresses the need to decarbonize the rail industry by advancing hydrogen engine technology for both current and future locomotives.*
> — ORNL distinguished researcher **Josh Pihl**

The project's initial goal is to displace up to 60 percent of diesel fuel with hydrogen and to create a retrofit option for the more than 25,000 locomotives already in use, which have life spans of 30 years or more.

Components of the train engine will be designed to run on both diesel and hydrogen initially, with the goal to fully replace diesel for next-generation locomotives. Image credit: Carlos Jones, ORNL

ORNL will work with Wabtec and Argonne to develop new hardware for the next generation of engines. Argonne will develop a modeling framework to study the combustion and emission control strategies used in hydrogen engines; simulation software will predict the behavior of engines when operating conditions change and hardware is modified. This will enable researchers to better understand what drives engine efficiency and reduces emissions.

"We are excited to be a part of this collaboration because it addresses the need to decarbonize the rail industry by advancing hydrogen engine technology for both current and future locomotives," said Josh Pihl, an ORNL distinguished researcher and group leader for applied catalysis and emissions research.

"It is also a perfect example of how a DOE-funded collaboration between industry and national laboratories can accelerate the development and commer-

A single-cylinder locomotive engine was installed at DOE's National Transportation Research Center at ORNL to study the integration of hydrogen as an alternative fuel source for diesel-powered railways. Image credit: Carlos Jones, ORNL

cialization of technologies to help reduce carbon emissions from transportation."

Hydrogen can be produced from clean energy sources such as solar and wind. Scientists have studied hydrogen-powered vehicles for decades, but it's a relatively new area of research in railway applications. Although hydrogen as a fuel has many advantages, it can ignite quickly, causing engine knock and backfiring. ORNL will ensure a safe, efficient and clean operation when it's introduced into the locomotive engine.

"Hydrogen burns very quickly, so one of the things we don't want to happen is engine knock, where it starts burning before you're ready for it to burn, because that can damage the engine or just give you nonoptimal performance," said ORNL's Dean Edwards, lead researcher on the project.

Edwards said the Wabtec collaboration aims to eventually develop combustion technology with up to 100 percent hydrogen and other low-carbon fuels. The goal is to design train engines that will deliver the same power, range and cost-effectiveness as current diesel technology. The research team will continue to alter engine hardware to increase the amount of hydrogen that can be used, eventually completely replacing diesel in new locomotives.

In addition, future research on alternative fuels for locomotives could incorporate renewable diesel or biodiesel to further reduce emissions. Each diesel-powered locomotive that is converted to a zero- or low-carbon energy source is anticipated to save up to 5.6 million pounds of carbon dioxide per year.

Blockchain helps increase electric grid resiliency

by S. Heather Duncan
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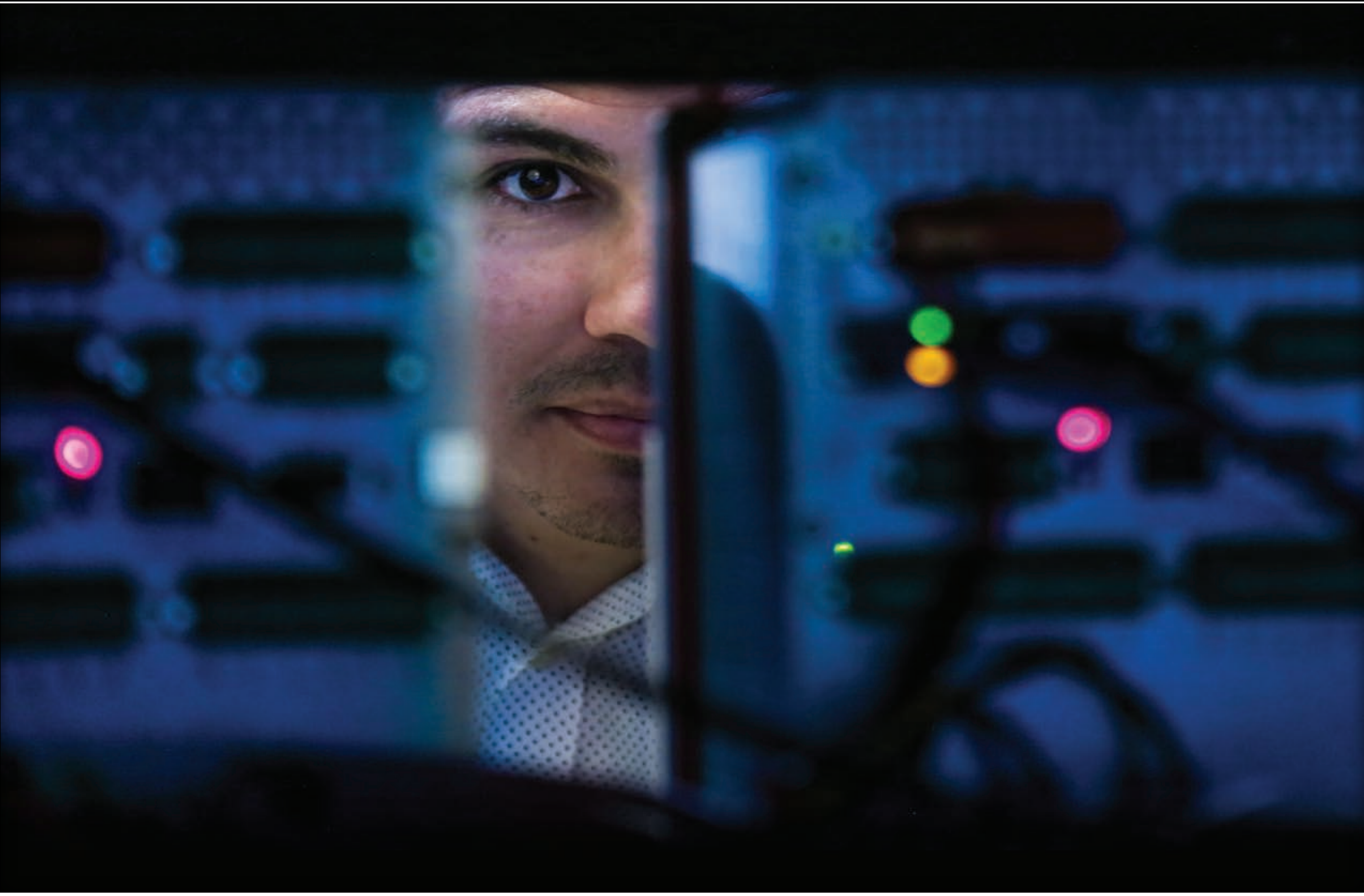
Although blockchain is best known for securing digital currency payments, ORNL researchers are using it to track a different kind of exchange: validating communication among devices on the electric grid.

The project, the first of its kind, is part of the ORNL-led Darknet initiative funded by the Department of Energy Office of Electricity. The objective of this initiative is to secure the nation's electricity infrastructure by shifting its communications to increasingly secure methods.

Cyber risks have risen in concert with increasing two-way communication between grid power electronics equipment and new edge devices. These devices range from solar panels to electric car chargers and intelligent home electronics. By providing a trust framework for communication among electrical devices, an ORNL research team led by Raymond Borges Hink is increasing the resilience of the electric grid. The team developed a frame-

From left, Emilio Piesciorovsky, Aaron Werth, Gary Hahn and Raymond Borges Hink test their blockchain-based validation system for grid communications in DOE's Grid Research Integration and Deployment Center at ORNL. Image credit: Genevieve Martin, ORNL



A team led by Raymond Borges Hink has developed a method using blockchain to protect communications between electronic devices in the electric grid, preventing cyberattacks and cascading blackouts. Image credit: Genevieve Martin, ORNL

work to detect unusual activity, including data manipulation, spoofing and illicit changes to device settings. These activities could trigger cascading power outages as breakers are tripped by protection devices.

"This framework gives us a totally new capability to rapidly respond to anomalies," Borges Hink said. "In the long run, we could more quickly identify an unauthorized system change, find its source and provide more trustworthy failure analysis. The goal is to limit the damage caused by a cyberattack or equipment failure."

The approach uses tamper-resistant blockchain to spread configuration and operational data redundantly across multiple servers. The data and equipment settings are constantly verified against a statistical baseline of normal voltage, frequency, breaker status and power quality. Equipment settings are collected at frequent intervals and compared to the last verified configuration saved in the blockchain. This allows rapid recognition of when and how settings were changed, whether those changes were authorized and what caused them.

"Our system helps determine in near-real-time whether a fault was triggered by a cyberattack or induced by natural events," Borges Hink said. "This is the first implementation of blockchain enabling this kind of data validation between a substation, a control center and metering infrastructure."

This kind of monitoring requires the processing of a vast amount of information. The blockchain uses a cryptographic method called hashing in which a mathematical computation is performed on the bulk data to represent it as numbers in the blockchain. This saves energy and reduces the space needed to store data. The blockchain processes thousands of transactions per second for each intelligent grid device, thus validating the contents.

Researchers demonstrated the framework in a test bed at DOE's Grid Research Integration and Deployment Center at ORNL. Built under the leadership of Emilio Piesciorovsky, this advanced protection lab uses commercial-grade hardware in a closed electrical loop to mimic the architecture of a real substation. The set-up provides a low-risk way to simulate cyberattacks or accidental misconfigurations. The team's validation framework could detect both. Researchers are extending the approach to incorporate communications among renewable energy sources and multiple utilities.

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.

Paul Cuillier

Graduate student, Neutron Scattering Division
Ph.D. student, Materials Science and Engineering, the Ohio State University
Hometown: Tucson, Arizona

What are you working on at ORNL?

I am using neutron total scattering measurements to train machine learning interatomic potentials for solid-state battery materials. We can apply these models to help interpret experimental results, simulate data to guide future studies, and conduct in silico experiments to accelerate materials design.

What would you like to do in your career?

I want to continue working at the interface between experimental and computational research, ideally in a setting like a national user facility where I can support a variety of research efforts.

Why did you choose a career in science?

I like solving puzzles that require working within constraints or combining concepts in new ways. A career in science is a great opportunity to do this daily while contributing to a better world.

Si Athena Chen

Postdoc, Chemical Sciences Division
Ph.D., Geosciences and Biogeochemistry, Pennsylvania State University
Hometown: Huanggang, Hubei Province, China

What are you working on at ORNL?

My research focuses on understanding the role of impurity ions on the crystallization of minerals using in situ X-ray/neutron scattering and high-resolution chemical imaging techniques. My interests include understanding crystal nucleation and growth, functional material synthesis and engineering, and crystal structure modeling.

What would you like to do in your career?

I find pleasure in working within a friendly and collaborative atmosphere, and I gained lots of knowledge in my first year as a postdoc. My desired career path involves working as a research scientist or beamline scientist at national laboratories.

Why did you choose a career in science?

There are moments when I believe that excelling in science also translates to success in other areas. My scientific background has endowed me with the skills to learn quickly, the courage to explore new life experiences, and the perseverance to achieve excellence. Engaging in science has a positive impact on my life.

Indranil Roy

Postdoc, Material Science and Technology Division
Ph.D., Mechanical Engineering, Lehigh University
Hometown: Bardhaman, India

What are you working on at ORNL?

My research uses computation to model the solidification of materials for complex processes such as additive manufacturing. This work provides a better understanding of a material's microstructural evolution, which will guide us for better alloy design and processing of robust materials.

What would you like to do in your career?

I would like to become a scientist working on real-life scientific challenges. ORNL has the resources I need to create scientific impact, and the people here are experts. Through teamwork, we can solve problems together.

Why did you choose a career in science?

I have always been intrigued by the process of solving challenging problems through critical thinking and with rigorous analysis. My training and prior experience in science and engineering give me immense satisfaction in solving real-life problems.

Subhamay Pramanik

Postdoc, Chemical Sciences Division
Ph.D., Chemistry, Guru Nanak Dev University, India
Hometown: Malda, West Bengal, India

What are you working on at ORNL?

My research involves the preparation of novel organic compounds and redox-active multidentate ligands for selective separation of rare earth elements using spectroscopic and analytical techniques. My work will help in discovering new strategies and methods for environmentally friendly and efficient extraction of lanthanides from their ores.

What would you like to do in your career?

I would love to resolve massive separation challenges of lanthanides and actinides since they have a huge role in the U.S. economic, energy and national security spheres. I want to use my synthetic organic chemistry expertise to develop materials and technologies to address these real-world challenges.

Why did you choose a career in science?

From my childhood, I wanted to become a scientist, which led to me becoming a chemist. I always enjoyed science classes with lots of different colors and natural products. Learning new ideas and brainstorming to solve problems always intrigued me.

Sreya Paladugu

Graduate student, Neutron Scattering Division
Ph.D. student, Materials Science and Engineering, University of Tennessee, Knoxville
Hometown: Fair Lawn, New Jersey

What are you working on at ORNL?

Through my fellowship at ORNL, I am studying hazardous-gas interactions with nanocatalysts using a new gas handling system at the Nanoscale Ordered Materials Diffractometer beamline at the Spallation Neutron Source. The end goal of this project is to extract design strategies for more robust, efficient and industrially relevant catalysts.

What would you like to do in your career?

Nanomaterials have enormous potential for creating innovative solutions. I hope to continue pursuing research in this area and find new ways to apply my experience in structure-property relationships in nanomaterials to advance our understanding of nanomaterials and their applications and make a positive impact on society.

Why did you choose a career in science?

I chose to pursue a career in materials science and engineering because I am fascinated by the unique properties that materials exhibit at the nanoscale and how these properties can be tuned for a diverse range of applications such as drug delivery, batteries and catalysis.

Mark Robertson

Graduate student, Neutron Scattering Division
Ph.D. student, Polymer Science and Engineering, University of Southern Mississippi
Hometown: Pensacola, Florida

What are you working on at ORNL?

My research uses neutron scattering to study how poly- and perfluoroalkyl substances, or PFAS, an emergent class of environmental contaminants, interact with porous materials at a molecular level. The goal of the research is to enable efficient removal of PFAS from the environment by understanding their fundamental assembly behaviors.

What would you like to do in your career?

After completing my Ph.D., I would like to continue performing research in an academic setting. More specifically, I'm interested in becoming a research professor where I can work directly with the next generation of scientists to promote environmental sustainability.

Why did you choose a career in science?

I enjoy continuously learning about the world around me, which led me toward a career in science. Science provides me the daily opportunity to think critically about puzzles in my research, while also acting as a leader for younger scientists, which I find very rewarding.

Katharine "Kay" Way. Image courtesy AIP Emilio Segrè Visual Archives, Wheeler Collection

Kay Way: The mother of nuclear data

by Jim Pearce
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In 1942, Katharine (Kay) Way was teaching physics at the University of Tennessee when a former professor recruited her to join the top-secret Manhattan Project at the University of Chicago.

Working at UChicago's now-legendary Metallurgical Laboratory under future Nobel prize-winner Eugene Wigner and alongside Alvin Weinberg — who would go on to be ORNL's longest-serving lab director — Way spent much of her time analyzing neutron flux data from Enrico Fermi's nascent nuclear reactor designs.

These efforts led to the world's first nuclear reactor, which was hidden under the stands at Stagg Field, the university's old football stadium.

While at UChicago, Way also teamed up with Wigner to study the problem of "reactor poisoning" — a condition that occurs when byproducts of nuclear reactions absorb so many neutrons that they slow or stop the chain reaction that powers the reactor. This work became known as the "Wigner-Way approximation for fission product decay."

"When Wigner moved to Oak Ridge in 1945 to become the laboratory's director of research, he brought a group of colleagues with him, including Kay Way and Alvin Weinberg," said Lee Riedinger, a retired University of Tennessee physics professor who has also served at ORNL's deputy for science and technology.

A crucial suggestion

In September of 1945, several of Way's friends and colleagues held a dinner for her.

"It was at that dinner," said Riedinger, "that she apparently suggested to University of Tennessee physics professor Bill Pollard and Kenneth Hertel, head of UT's Physics Department, that they should do something in Oak Ridge like the universities around Chicago were doing — that is, forming an organization to make use of the Manhattan Project facilities in Chicago, which eventually became Argonne National Laboratory."

Way's suggestion led to formation of the Oak Ridge Institute of Nuclear Studies, which became Oak Ridge Associated Universities.

"ORINS became Bill Pollard's baby," Riedinger said, "but it was Kay Way's suggestion that gave Pollard the idea that he then carried out. There are people who say that the existence of ORINS was an important part of the decision to keep Oak Ridge's Manhattan Project facilities funded."

Focusing on nuclear data

"While at Oak Ridge, Way continued her work with fission product decay and began to focus more intently on collecting and organizing data related to nuclear reactions," Riedinger said.

"After the Manhattan Project, she got more interested in the data — the nature of the nuclei that you make when uranium fissions. That was important. People realized that if you're going to work on fission, you've got to know what the fission products are and what radioactivity is associated with them. Kay Way realized that, and gathering data on the properties and radioactive decay of nuclei became the focus of her career."

In 1949, Way left ORNL to head up the new nuclear data group at the National Bureau of Standards — known today as the National Institute of Standards and Technology — in Washington, D.C. In 1953 she convinced the National Academy of Sciences' National Research Council to create the Nuclear Data Project, which eventually gave birth to the seminal nuclear data journal *Nuclear Data Sheets* in 1964.

Later, in 1964, Weinberg, convinced Way to move back to Oak Ridge, where she headed up the lab's nuclear data group and continued to oversee *Nuclear Data Sheets*. In 1965, she helped launch a second nuclear data journal, Atomic Data and *Nuclear Data Tables*.

In 1968, Way retired from ORNL, took a position at Triangle Universities Nuclear Laboratory in Durham, North Carolina, and became an adjunct professor at Duke University. However, her presence was still strongly felt in the field of nuclear data as she continued as editor of *Nuclear Data Sheets* until 1973 and *Atomic Data and Nuclear Data Tables* until 1982.

"That was her passion"

"The database that Kay produced was, and is still, very important," Riedinger said, "not only to researchers doing fundamental nuclear physics experiments, but also to people building nuclear reactors, people doing nuclear forensics and people working in any field that relies on nuclear instruments or nuclear fission."

"She started collecting nuclear data just after the Manhattan Project ended. She built the research group. She started the nuclear data journals that we depend on today. She built the field of nuclear data. That was her passion."

What was it like to be a woman in the physical sciences in 1956? Kay Way (center) was among the attendees at the Conference on Nuclear Masses and Their Determination, held at the Max Planck Institute in Mainz, West Germany, from July 10-12, 1956. Image courtesy AIP Emilio Segrè Visual Archives, Wheeler Collection

Welcome to Research Insights

Additive Manufacturing the Future, Part I: Applications for Additive Manufacturing

ORNL Review is pleased to present the fifth issue of *Research Insights*, a collection of research articles from our scientific and technical staff. *Research Insights* was created to showcase the world-leading science being performed at ORNL, with each issue addressing an important theme.

This issue highlights recent advances by ORNL staff in additive manufacturing. Manufacturing represents 12 percent of gross domestic product, provides nearly 13 million jobs and accounts for a quarter of energy use. Therefore, innovations in sustainable manufacturing are central to the nation's prosperity and security, and world leadership in additive manufacturing can lead to substantial job creation in the United States.

During the last decade, ORNL has developed a substantial fundamental and applied research program as part our Additive Manufacturing Initiative. Within this initiative, ORNL is working to improve energy-efficient metal and polymer additive methods, reduce the wastage of feed materials, attain properties comparable to conventionally manufactured parts, lower cost, develop rapid prototyping and sustainable recycling, create automated manufacturing and tools for in-situ monitoring, take novel 3D printing approaches, improve functionality, and create new high-efficiency applications.

Articles in this issue of *Research Insights* reflect these efforts, addressing technologies that develop software packages for bridging the gap between design, print path planning and visualization; use neutrons to understand and mitigate residual stress during printing; predict and control the melt pool path during parts manufacturing; fabricate lightweight titanium aluminide alloys with high strength and improved corrosion resistance compared to nickel-base superalloys; and use artificial intelligence techniques to visualize the additively manufactured parts through X-ray computed tomography.

The articles presented in this issue of *Research Insights* represent a small fraction of the ORNL research portfolio dedicated to helping achieve the nation's additive manufacturing goals. We hope that you enjoy reading the exceptional work being performed by ORNL staff.

Additive Manufacturing of Nuclear Fuel

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INTRODUCTION

Nuclear power is the only current technology that can meet the nation's baseload clean energy needs. However, building new reactors in today's economy carries significant risk, especially when considering large light-water reactors (LWRs) with significant capital investment requirements. For example, the cost for Vogtle Units 3 and 4 (>1,100 MWe each) has now exceeded $30B. Small modular reactors (SMRs, <300 MWe) and microreactors (<20 MWe) are being considered to reduce onsite construction costs and to target a wider range of energy markets. Their success will rely heavily on the reduced costs of factory manufacturing and assembly, increased efficiencies in power conversion offered by advanced materials, and complex geometries enabled by additive manufacturing (AM). AM could also help reduce operation and maintenance costs by integrating placement of sensors into the component manufacturing process. Sensors embedded at strategic locations would allow the internal health of components to be monitored, ultimately preventing costly unplanned shutdowns and reducing the need for time-consuming visual examinations..

BACKGROUND

The fuel element—the most critical component of any nuclear reactor—contains the fissionable material, typically U. The fuel generates heat via fission, contains radioactive fission products, and safely rejects heat to the reactor's coolant. Nuclear fuel designers are always seeking ways to increase the U density while maintaining or improving acceptable performance under normal operation, anticipated operational occurrences, and design-basis accident scenarios. Conventional LWRs use monolithic UO_2 ceramic pellets uniformly enriched in ^{235}U (<5 wt%) and contained in a cylindrical Zr-alloy cladding. This geometry maximizes the U density and is amenable to large-scale fabrication processes. However, recent efforts to extend the maximum allowable fuel burnup (operational lifetime) to increase economic efficiencies have been stunted by technical challenges caused by localized nonuniform burnup distributions across the fuel that can lead to severe fragmentation under certain accident conditions. AM could enable isotopic and compositional gradients within the fuel to help minimize spatial variations in burnup and can also provide other neutronic advantages such as integrable burnable absorbers [1]. Isotope production targets share similar interests in isotopic/compositional gradients to increase yields.

RESULTS

Drop-in replacements for current LWR fuel. The licensing and qualification process for new nuclear fuel forms is long and complex, often taking more than 20 years [2], even for relatively minor changes in the fuel. This schedule does not include the time and cost required to modify various reactor systems or infrastructure for fabricating, inspecting, and handling the fuel if the geometry were to change significantly. Therefore, the current fleet of LWRs would benefit from a drop-in replacement that could help mitigate high burnup fuel fragmentation concerns and lower fuel operating temperatures. The latter reduces the effects of thermally driven processes such as diffusion and release of radioactive fission products from the ceramic fuel pellets, which increases the internal pressure of the fuel rod and can lead to costly fuel failures.

Figure 1 summarizes potential drop-in replacements for current LWR fuel vs. reference UO_2 pellets (Figure 1a). The simplest change would be to use the same UO_2 pellet but incorporate zoned ^{235}U enrichment to minimize local peaking in the spatial burnup profile (Figure 1b). For example, reducing the ^{235}U enrichment at the periphery of the pellet and increasing the enrichment in the center would help create a more uniform burnup profile if varying enrichment zones could be selectively created using AM.

Although zoned enrichment is in the conceptual stage at this writing, parallel efforts have been made to enhance the effective thermal conductivity of the fuel to reduce fuel temperatures by adding more conductive materials. Other organizations have demonstrated improved thermal conductivity of UO_2 pellets using homogenous additions of Mo (Figure 1c) [3]. Taking this one step further, 3D conductive Mo inserts have been designed to insert in UO_2 to enhance the directional heat transfer and improve radial heat rejection to the reactor coolant. The simplest case involved optimization of a series of Mo rods and plates (Figure 1d) [4]. ORNL has proposed and patented more complex structures (Figure 1e) that involve additively manufacturing a conductive tree-like structure that would be integrated into the fuel pellet during manufacturing [5]. Recent efforts [6] have leveraged unconstrained genetic algorithms to selectively place Mo in the locations that will most effectively reduce the maximum fuel temperature. Ultimately, this work seeks to determine a compromise between the lower temperatures resulting from optimally placed Mo vs. the loss of U that is displaced by Mo and the feasibility of fabricating more complex additively manufactured Mo structures.

AM of fuel cladding to enable new UO_2 fuel geometries. Precise grinding of UO_2 pellets to achieve tight geometric tolerances is a critical step in the fuel fabrication process. Fuel temperature and performance are dictated by the gas gap (or contact) between the pellet and cladding. Oversizing the pellet diameter risks stressing the cladding as the pellet expands and eventually

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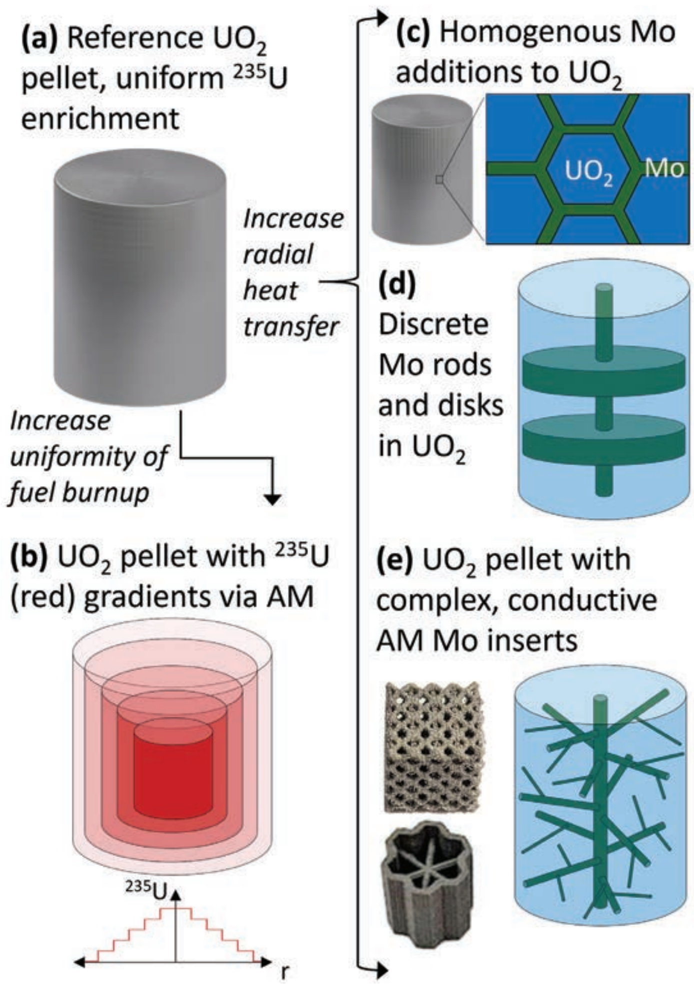

Figure 1. Left column – (a) current LWR fuel pellets, and (b) a drop-in replacement that comprises UO_2 pellets with ^{235}U gradients via AM to flatten burnup profile (Credit: A. Malin); right column – UO_2 pellets with enhanced thermal conductivity: (c) homogenous additions of Mo, (d) simple Mo rods and plates, and (d) complex Mo structures enabled by AM to most effectively enhance radial heat transfer (Credit: C. Petrie).

contacts the cladding, which creeps down under the pressure of the reactor coolant. Undersizing the pellet diameter reduces the fuel loading (affects economics and cycle length) and increases the fuel temperature because of poor heat transfer through large gas gaps between the fuel and cladding. Although grinding cylindrical pellets is expensive, grinding this geometry is still far simpler than grinding more complex shapes that may otherwise be more advantageous for reactor designers, at least from a uranium loading perspective. If not for concerns with geometric tolerances, moderately complex UO_2 geometries could be fabricated simply by modifying the die used for pressing. However, the post-pressing sintering process required to increase pellet density results in significant pellet shrinkage, and precise dimensional control cannot be achieved without subsequent grinding.

One approach to achieving moderately complex UO_2 fuel geometries without requiring expensive grinding operations is to use AM to incorporate special features into the surrounding fuel cladding to relax the tolerances on the pellet dimensions. The US Department of Energy Office of Nuclear Energy (DOE-NE) pursued this concept early in the development of the Transformational Challenge Reactor (TCR) fuel form (see Figure 2) [7].

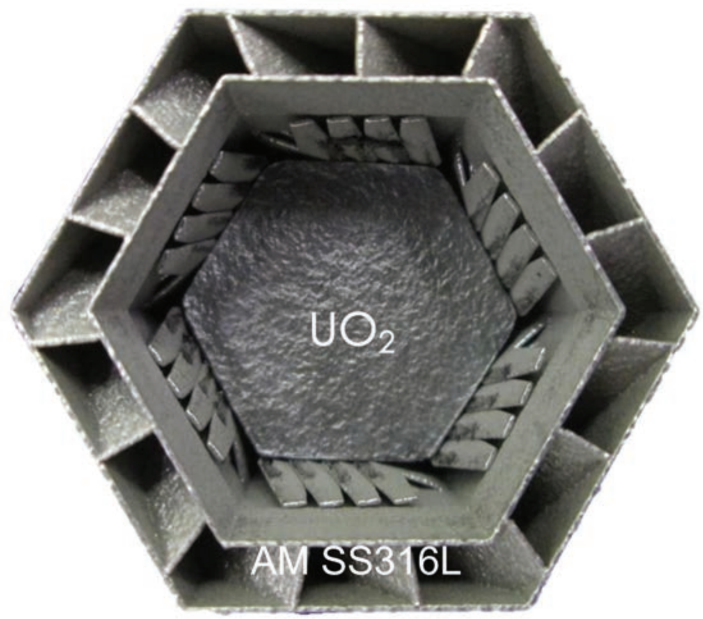

Figure 2. AM SS316L can with compliant fin features to increase allowable dimensional tolerances on the hexagonal UO_2 pellet and outer channels to encourage coolant mixing and enhance heat transfer. (Adapted from Betzler et al.) [7].

In this example, a hexagonal pellet was fabricated via traditional pressing and sintering. The surrounding metal can was 3D printed from 316 stainless steel, and two features were incorporated to enhance fuel performance and increase the tolerance of the pellet dimensions [8]. Thin, compliant structures were printed on the inner surfaces of the can to improve heat transfer through the pellet-can gap while compressing as needed to accommodate dimensional tolerances in the pellet without significantly stressing the primary can walls. In addition, the outside of the can included printed channels to direct coolant flow and enhance turbulent mixing to improve heat transfer. These features could help reactor designers increase the uranium loading in the reactor core by enabling new geometries that were either not possible or prohibitively expensive using conventional manufacturing processes.

High-performance plate fuels. Plate fuels are commonly used in research and test reactors that operate at relatively low temperatures but at extremely high burnups. These fuels have typically been fabricated by dispersing fine uranium-bearing powders in a metal matrix and cladding the fuel meat with solid metal plates. The fuel loading generally varies over the length of the fuel element to reduce power peaking that would otherwise exist near the center of the fuel plate where the neutron flux is highest. Therefore, controlling and understanding the local fuel loading has important implications on fuel performance and safety. The higher the uncertainty in the fuel loading, the more conservativism is needed in operating the fuel, thus limiting reactor performance. Mechanical mixing of uranium-bearing powder with matrix material results in significant uncertainties that limit the performance of plate-type fuels.

ORNL is pursuing hybrid manufacturing processes such as ultrasonic additive manufacturing (UAM) to allow for a more controlled, ordered arrangement of fuel and for strategic placement of embedded sensors within relevant materials (e.g., Zr-alloys) to monitor local fuel temperatures and strains [9, 10]. In this concept (Figure 3), UAM is first used to build up the fuel cladding by layering thin foils. Then, subtractive computer numerical control milling is performed to machine cavities or channels that contain fuel and/or sensors placed in precise locations. Subsequent UAM layering of additional foils embeds the fuel and/or sensors within the fuel matrix and builds up an additional cladding on top of the fueled region. UAM is advantageous because it is a solid-state, melt-free process that minimizes damage to the fuel and sensors during embedding. Furthermore, precise subtractive operations could greatly improve the understanding of fuel loading in each element. Successful development of this fuel form could increase the neutron flux and/or cycle length of the nation's research and test reactors to benefit a wide range of experiments spanning neutron scattering, isotope production, and testing of experimental nuclear fuels and materials.

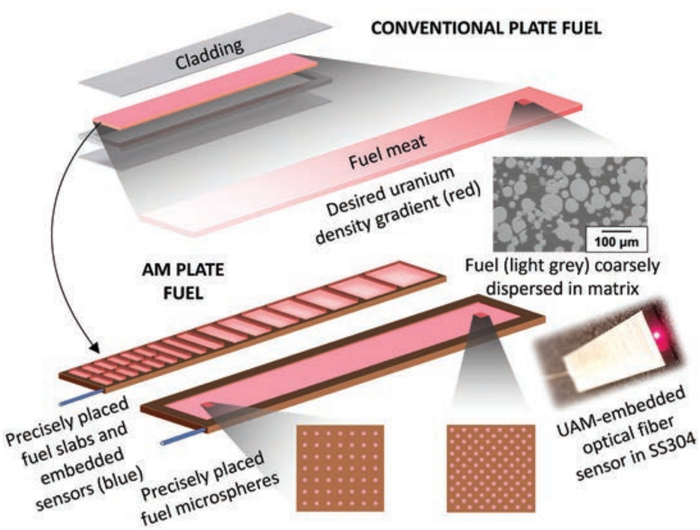

Figure 3. Illustrations of conventional plate fuel vs. a conceptual fuel form with highly controlled placement of fuel and embedded sensors enabled by UAM (Credit: A. Malin).

Transformational particle fuel concepts. Perhaps the most exciting advancement in the nuclear fuels community has been ORNL's recent development of TCR fuel [11, 12]. This patented fuel fabrication process [13] leverages the ability of traditionally manufactured uranium nitride (UN) tristructural-isotropic (TRISO) fuel to contain radioactive fission products, but it also enables full geometric freedom while greatly enhancing uranium loading within the fuel. TRISO particles comprise sub-millimeter uranium-bearing spheres (or kernels) with multiple coating layers (see Figure 4) that allow the fuel to expand without compromising the ability of the layers to retain fission products. The TCR fuel has a complex cog shape that is created by binder jet 3D printing a radiation-tolerant SiC shell which is then filled with UN TRISO fuel particles with maximum geometric packing. The remaining space is filled with loose SiC powder. The final step involves densifying the entire fuel form with crystalline SiC using a chemical vapor infiltration (CVI) process to prevent the need for hot rolling, uniaxial pressing, or other rigorous processes. This approach enables higher packing fractions (higher U density) to increase economics without sacrificing safety or other fuel performance metrics. Moreover, placing sensors prior to loading TRISO particles allows the sensors to be embedded within the SiC matrix during CVI [14, 15]. This allows limiting fuel centerline temperatures to be monitored during reactor operation, which could further reduce the conservatisms introduced when relying on models to estimate fuel temperatures during operation.

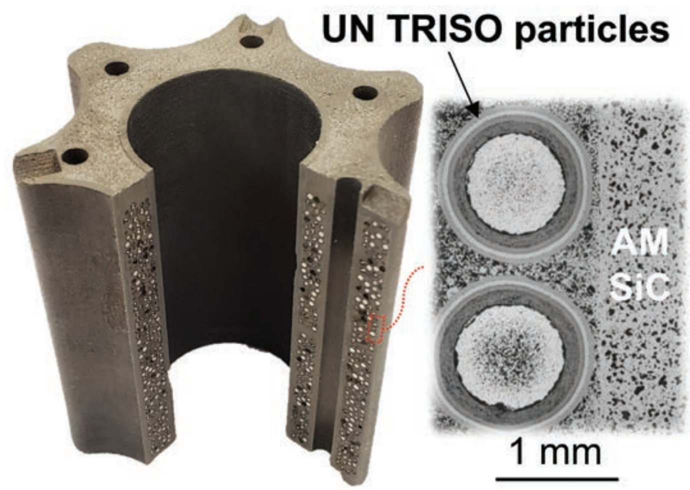

Figure 4. Sectioned TCR fuel cog containing a dense packing of UN TRISO particles in a SiC matrix within a complex, 3D printed SiC shell [12]. The image on the right shows the interface between UN TRISO particles and the outer binder jet printed SiC shell. (Reprinted from *J. Nucl. Mater.* 580, C. Petrie et al., Copyright 2023, used with permission from Elsevier).

CONCLUSIONS

Nuclear fuels may benefit from AM more than any other component in a nuclear reactor, but the industry is only beginning to realize the potential impact. ORNL has taken the lead on the design and fabrication of these AM fuel forms, with examples including drop-in replacements for current commercial and research/test reactor fleets; expanded UO_2 pellet geometries enabled by complex features incorporated into the cladding via AM; and transformational concepts for integrating densely packed TRISO fuel particles into highly complex, robust SiC matrices. This work is only the beginning of what can be achieved by designing nuclear reactors free from the traditional constraints imposed by fuel fabrication limitations.

IMPACT

Although these AM fuel concepts were only introduced within the past few years, the nuclear industry has been quick to pursue these concepts. Numerous commercial LWR fuel vendors and utilities are exploring the economic incentive offered by enrichment or poison zoning. Ultra Safe Nuclear Corporation has licensed multiple ORNL patents related to the TCR fuel form and supporting technologies. The BWXT Advanced Nuclear Reactor will utilize a similar TCR fuel form that is being developed under DOE-NE's

Advanced Reactor Demonstration Program. The coming decade will undoubtedly see these and similar approaches being leveraged to improve fuel performance and reactor safety to reduce the world's carbon footprint and increase energy security.

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3D Printing of Natural Fiber-Polylactic Acid Composites to Decarbonize Structural Composites

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INTRODUCTION

New plastic composites are in high demand in the construction, manufacturing, and transportation sectors to meet structural strength specifications while minimizing environmental and health hazards. Composites are made by blending powders or fibers in plastics to obtain the desired properties in the final product, including load-bearing capacity, stiffness, surface appeal, and weight. Plastics offer several benefits, such as low density, high strength, hydrophobicity, and corrosion resistance, thus adding to their appeal. Natural fibers derived from lignocellulosic biomass sources like wood, straw, jute, hemp, and coconut coir are blended with plastics, yielding composite panels that are lightweight, durable, low-cost, and visually appealing [1]. However, the plastics used in current commercial applications to make these composites are synthesized from highly carbon-intensive, petroleum-derived monomers. They are not recycled multiple times to realize their full potential before they lose their mechanical strength. They can eventually accumulate in large quantities in earth or ocean bodies for long periods of time because of their lack of biodegradability or compostability. Some examples of these petroleum-derived plastic polymers are polyethylene, polypropylene, and polyamide (nylon). The preponderance of accumulated plastics makes it is necessary to utilize plastics with lower carbon footprints that can be recycled or degraded more quickly at the end of their use cycles [2].

Polylactic acid (PLA) has emerged as an alternative to conventional thermoplastics for composite manufacturing. PLA is made from the polymerization of lactic acid, a fermentation product of plant sugar fermentation. It has a lower carbon footprint than plastics like polyethylene and nylon, and it can be composted in industrial facilities at the end of its use cycle. A major benefit of PLA is that it can be easily used to manufacture composites through additive manufacturing (AM) or 3D printing. 3D printing of thermoplastics involves layer-by-layer deposition of molten plastic polymer that bonds on cooling to build an object of a specified design [3]. 3D printing provides advantages such as mold-free fabrication, the ability to manufacture complex, customized products, scalability, and localized manufacturing. Natural fibers from wood, grasses, sawdust from mills, paper waste, cardboard, fruit peels, and forest residues are low-cost, widely available renewable fillers to make 3D-printed PLA composites [1].

ORNL and its partners, including the University of Maine and the University of Tennessee - Knoxville, have led the efforts in 3D printing of natural fiber–PLA composites at benchtop to demonstration scale in the United States (Figure 1) [4]. Scientists with niche expertise across several ORNL divisions collaborated to investigate the properties of natural fibers and PLA, manufacturing conditions, and composite properties. Based on these efforts, these PLA composites can now be used to replace conventional thermoplastic composites to reduce the environmental footprint at the industrial scale.

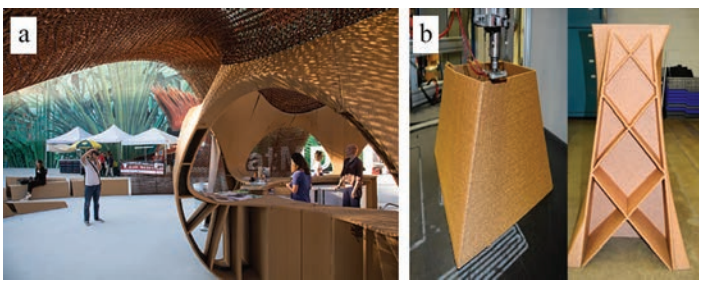

Figure 1. (a) 30-meter-long bamboo-PLA installation at Design Miami 2016 printed at ORNL's Manufacturing Demonstration Facility; (b) large-scale 3D printing process using poplar / PLA composite (left photo), and a completed 3D printed podium base (right photo: back of podium base). (Credits: (a) ORNL internal images, (b) Reprinted (adapted) with permission from Zhao et al. [6] Copyright 2019, American Chemical Society).

BACKGROUND

Poplar hardwood is a fast-growing sustainable woody lignocellulosic biomass that has been used as a natural fiber in several of these studies [5,6]. Biomass from poplar trees offers high carbon savings because of its relatively low growing resource consumption. Moreover, ORNL has an extensive collection of poplar logs from trees grown in a common garden for the study of gene function. The logs are used to study the impact of wood variety on the mechanical strength of printed composites. A standard poplar was used to study how wood content in wood–PLA composite affects biomass milling methods, biomass particle size, and printing conditions. After optimizing these conditions, 200 poplar variants were used to print 200 wood–PLA composites under the same manufacturing conditions to understand the role of biomass structure on the composite's mechanical properties.

Improved mechanical load distribution within the composite can improve the load-bearing capacity of biomass-PLA composites. This effect is achieved by modifying biomass surfaces with additives that enhance the bonding between biomass and PLA. Epoxy modification of pine softwood [7] and the addition of lysine amino acid to poplar hardwood [8] were carried out to improve interfacial bonding and properties.

Cellulose nanofibers can be obtained from biomass through chemical or mechanical means, offering outstanding specific properties. However, they have bonding issues similar to those of wood particles when they are used in polymer composites. ORNL made various modifications for use of cellulose nanofibers derived from softwood pine in thermoplastic composites. Cardboard waste has also been analyzed as a source of cellulose nanofiber for use in low-cost cellulose-PLA composites [9]. Such applications extend the use-cycle of cardboard, thus improving the circular economy of wood-based products.

RESULTS

3D printing of poplar wood–PLA composites. The following steps were used to make 3D printed composites: reducing the size of the biomass, melt blending the biomass with PLA, extruding the biomass-PLA blend to make filaments, and feeding the filaments into the 3D printer for printing.

Appropriate size reduction of biomass is important, as particle size affects the mechanical properties of the composites and controls the high-temperature flow behavior in the heating chamber and nozzle of the 3D-printer. Wood chips were milled into powders of different size ranges by knife, hammer, and ball milling. The fiber size distributions were controlled further by sieving. For benchtop 3D printers, biomass particle sizes should be below 200–300 μm to avoid clogging the printer nozzle [5]. Additionally, keeping the biomass particle sizes lower than 180 μm results in fewer voids in the composite [6].

Melt blending of biomass and PLA is an important step to achieve a homogeneous biomass distribution in the PLA matrix. Melt blending was performed using a compounding extruder that melted and blended the biomass-PLA mixture at 180–210°C. This well-mixed blend was then extruded in the same temperature range to create filaments. Filament diameter must be controlled to prevent overflow or underflow during printing. The presence of biomass in PLA increased the solidification rate of filament compared to neat PLA, and cooling rates were adjusted to obtain reasonable control over filament diameter. Figure 2 shows scanning electron microscopy (SEM) images of wood flour–PLA composites.

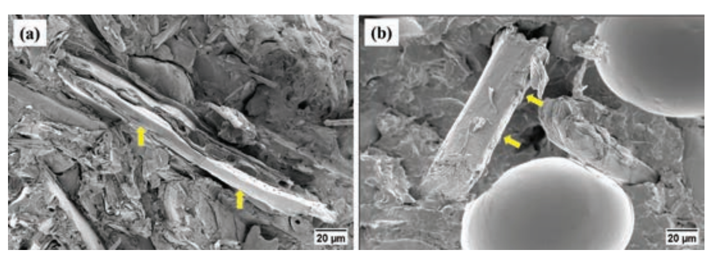

Figure 2. SEM images of wood flour–PLA composites; Biomass fibers in PLA matrix indicated by arrows. (Source: ORNL internal images).

Testing various wood contents in PLA showed that 3D printing was consistent and had no failures at 20 wt.% wood–PLA composites (80% PLA). Moreover, because increased presence of biomass in PLA increased the solidification rate, it was found that printing of the biomass-PLA composite at higher temperature (210–230°C) achieved better results than neat PLA, which can be printed at 180°C. At higher temperatures, the printing layer from the printer nozzle bonded to the lower layer before the molten material solidified, thus resulting in improved strength.

Two hundred poplar trees with various chemical compositions were used to study the impact of biomass structure on composite strength [5]. Tree logs were used to prepare 20% poplar wood–PLA composites by 3D printing. The results showed median tensile strength values at 48 MPa and Young's modulus at 3.6 GPa. For comparison, neat PLA thermoplastic has 50 MPa tensile strength and 2.8 GPa Young's modulus (Figure 3). Therefore, the addition of wood increased the stiffness (Young's modulus) by 30% without significantly sacrificing tensile strength. Moreover, a positive correlation between cellulose content of biomass and Young's modulus of composite was found, suggesting that using biomass with higher cellulose content can result in composites of higher Young's modulus.

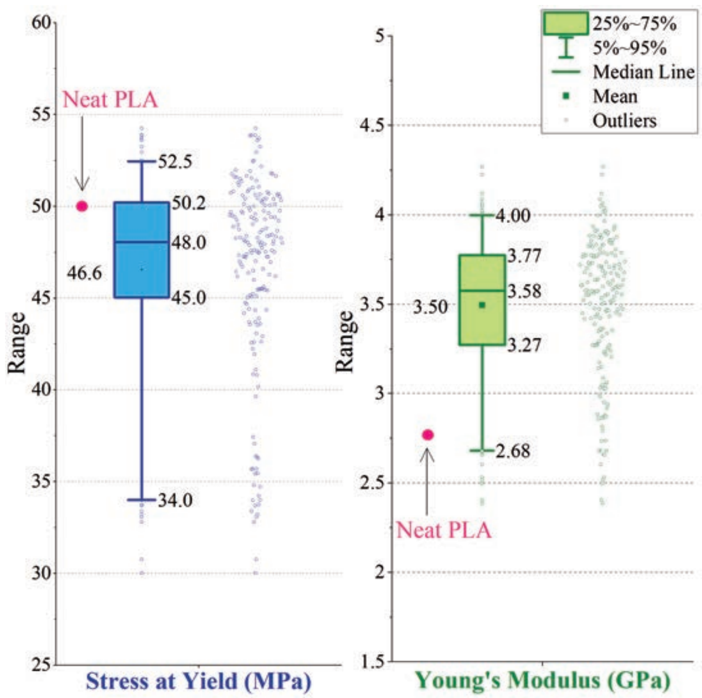

Figure 3. Tensile stress at yield, and Young's modulus of 20% wood–PLA 3D printed composites using 200 poplar trees to study the impact of biomass structure on properties of composites. Neat PLA (no wood) data shown for comparison. (Source: ORNL internal data).

Enhancing bonding between biomass and PLA by additives or chemical modification. When composites are subjected to mechanical loads, the load distribution between biomass fibers and the thermoplastic matrix plays a key role in determining the load-bearing capacity. Therefore, good bonding of biomass fiber surfaces with PLA is important. However, biomass is hydrophilic, and PLA thermoplastic is hydrophobic. This creates a mismatch between their surfaces that hinders good bonding. However, this can be overcome by surface treatment of biomass. With only 1 wt.% impregnation of pine wood fibers with epoxy, 30% pine wood–PLA composites could achieve high strength with 71 MPa tensile strength and 5.4 GPa Young's modulus [7].

In another work, the addition of just 0.1% lysine amino acid to poplar wood powder increased the Young's modulus of 20% wood–PLA composites by 68%. This effect was thought to be caused by better penetration of PLA polymer chains in biomass pores resulting from the presence of lysine [8].

Numerous aqueous reactions have been developed for compatibilization or modification of cellulose nanofibers without harsh solvents for low-energy high-performance composites. In a recent study, chemical modification of cellulose fibers with an aqueous vinyl laurate system improved the tensile strength and Young's modulus of their PLA-based composites by 38% and 71%, respectively [10].

Chitosan is a widely available natural biodegradable polymer that is recovered from the exoskeletons of crustaceans such as shrimp and crab waste. Adding a small amount (2.5 wt.%) of chitosan to PLA with 30 wt.% cellulose nanofibrils was found to increase stiffness by 39% compared to neat PLA while maintaining a high tensile strength, whereas the same amount of cellulose nanofibers without chitosan increased the stiffness of PLA by 25% but lowered its tensile strength [11].

Cellulose nanofibers from recycled cardboard for cellulose-PLA composites. Cellulose nanofibers from corrugated cardboard are an attractive resource for making cellulose–PLA composites because such cardboard costs only $108/ton, whereas bleached softwood pulp fibers from paper mills can cost $1,100/ton [9]. Cardboard biomass was pulverized and ground into disk refiners to obtain nanoscale cellulose fibers. Energy consumption in grinding of such cardboard cellulose fibers (1,200 KWh/megaton) was only 55% of that required for grinding of cellulose pulp from paper mills into nanofibers (2,200 KWh/megaton) [9] (Figure 4).

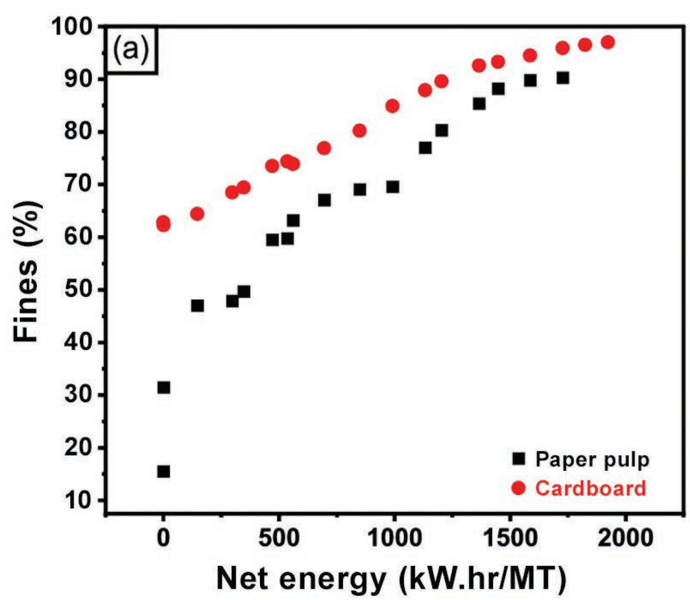

Figure 4. Net energy required to reach cellulose fines percentages for cardboard and paper pulp fibers. (Reprinted [adapted] with permission from Copenhaver et al. [9] Copyright 2021 American Chemical Society).

When cardboard cellulose nanofibers were used to make cellulose–PLA composites at 40% cellulose content, the Young's modulus of the composite (5.85 GPa) increased by 73% in comparison to neat PLA. This high strength was proposed to be caused by the presence of lignin polymer in the cardboard cellulose fibers that increases the fibers' surface hydrophobicity and improves bonding with PLA [9].

ORNL researchers conduct technoeconomic analysis (TEA) and life cycle analysis (LCA) to understand the costs and energy and carbon footprints of such 3D printed natural fiber–PLA composites. LCA calculators at ORNL can determine the energy consumption and CO_2 release from biomass production, harvest, storage, and delivery, as well as fiber processing operations like chemical treatments, refining and drying, and printing operations like melt blending, printing temperature, and printing time to understand the environmental impacts of these composites.

CONCLUSIONS

Adding 20% poplar wood to PLA increased the stiffness of 3D printed composites by 30% without sacrificing the load-bearing capacity in comparison to neat PLA thermoplastic. Impregnating biomass with low concentrations of additives like epoxy, amino acid, or chitosan improved the strength of the composites. This result was the outcome of better bonding between biomass and PLA, which improved the mechanical load-bearing distribution inside the composite. Using cardboard biomass waste to make composites reduced cost and energy consumption because of the lower cost of this biomass resource and the significantly lower energy requirements for refining it into nanofibers.

IMPACT

Incorporating biomass fibers to enhance the performance of PLA composites makes them feasible replacements for petroleum-derived plastics for large-scale AM. It reduces cost and increases material renewability. The use of plastics like PLA that are derived from plant sugars reduces the net CO_2 release in the environment. Because PLA is compostable and wood is biodegradable, these composites are more environmentally friendly than conventional thermoplastic composites.

The ability to 3D print such composites supports the advanced manufacturing capabilities in the United States. The composites made for 3D printing have high strength and stiffness and can be used to fabricate products for construction, infrastructure, transportation, and household needs. 3D printing of bio-based composites has been successfully demonstrated on a large scale at ORNL for applications such as tooling and specialty packaging. These large printed parts have also been shown to be recyclable, further reducing the embodied energy and environmental impact of PLA/biomass composites.

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Additive Manufacturing Facilitating Process Intensification of CO_2 Capture

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INTRODUCTION

Capture of carbon dioxide (CO_2) is needed to reduce anthropogenic greenhouse gas emissions to the atmosphere. Gas–liquid absorption in packed columns has been extensively studied for this purpose [1]. Significant drawbacks continue to prevent carbon capture from attaining commercial viability, including high energy penalty, which is estimated at 3.7 gigajoules (GJ) per tonne of CO_2 based on amine absorption [2]. Process intensification of point-source CO_2 capture has received extensive consideration as an option to minimize the energy penalty and cost. Additive manufacturing (AM) has already been proven as a means to achieve process intensification of CO_2 capture in gas–liquid–packed columns.

Over the past three years, Oak Ridge National Laboratory (ORNL) has shown that additively manufactured packing devices can be used to enhance mass transfer of CO_2 from the gas phase to the liquid solvent in packed columns, while transferring heat from the reactive gas–liquid fluids to a cooling fluid that is used to remove heat generated by the reaction between CO_2 and solvent molecules [3–7]. Both actions are critical in maintaining a high CO_2 removal efficiency. Because these packing devices carry out multiple functions, they have been termed process-intensification packing elements (PIPEs). PIPEs have been used to demonstrate CO_2 capture enhancements up to 25% for two different solvents compared to commercial packing, which is used simply for mass transfer enhancement [4–6].

Based on the encouraging results using additively manufactured PIPEs, the US Department of Energy (DOE) Office of Fossil Energy and Carbon Management and Advanced Manufacturing Office supported development of a CO_2 capture research platform at ORNL's National Transportation Research Center (NTRC) to further develop and scale up process-intensification devices based on AM for future industrial-scale applications for CO_2 capture. The new CO_2 capture platform includes a 4 m tall packed column measuring 0.3 m in diameter. The column is equipped with additively manufactured PIPEs measuring 0.3 m diameter and 0.4 m height, a solvent storage and delivery system, a solvent regeneration system, and a monitoring and control system. The CO_2 source for the research effort originates from a 100 kW natural gas–fueled generator with load and temperature control which produces realistic exhaust gas and load cycles representative of operation by industry partners such as the Tennessee Valley Authority (TVA), at the GW power plant scale. This work describes PIPE's current efficacy on bench-scale experiments and the ongoing work to advance to the pilot-scale column.

BACKGROUND

The Intergovernmental Panel on Climate Change (IPCC) reported growth in anthropogenic greenhouse gas emissions since 1990 [8]. By 2019, CO_2 emissions from fossil fuel power plants and industry sectors showed the largest growth, followed by CH_4 emissions. Significant reductions in CO_2 emissions (45% by 2030 and 100% by 2050) are urgently needed to meet international greenhouse gas (GHG) emission targets [9]. These goals can be achieved by developing novel CO_2 capture, utilization, and storage technologies.

Depending on the source of CO_2, capture can be identified as point-source or direct air capture. Point-source capture refers to removal of CO_2 from gaseous emissions, such as power generation related flue-gas or industrial emissions in which the CO_2 concentration is relatively high, >1%, compared to the atmospheric concentration of 0.04%. Alternately, direct air capture seeks to capture CO_2 directly from the air, as the name implies, and is considered a negative emissions technology because it directly reduces the atmospheric CO_2 concentration. The focus in this work is on point-source CO_2 capture either from power generation or industrial processes to avoid further increases in atmospheric CO_2 concentration. Reactive absorption using suitable solvents is a technology commonly used to capture CO_2 from point-source emissions. Several solvents have recently been investigated, including aqueous and nonaqueous or low-aqueous solvents (LASs). Some amine-based solvents include monoethanolamine (MEA), diethanolamine (DEA), and piperazine, while others are based on amino acids [10,11].

Common characteristics of these solvents are high pH, high CO_2 capacity, and exothermic reactions with CO_2, which indicates that the solvents will need thermal energy to release CO_2 molecules. Thus, as a solvent captures more and more CO_2 in an absorption column, for example, its temperature increases from the heat generated by the exothermic reaction with CO_2. As the temperature of the solvent increases, its ability to capture more CO_2 diminishes. In a CO_2 capture process, the objective is to keep the solvent's CO_2 capacity high, which can be achieved by cooling the solvent as it flows through the process equipment.

Columns with structured or random packing are commonly used for gas–liquid absorption on an industrial scale. The columns provide a high surface area for enhanced transport

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rates between the gas and the liquid phases, and the packing material is well wetted by the liquid solvent. Structured packing has the advantage of lower pressure drop, or lower resistance to fluid flow through the gas–liquid contactor, over random packing or other types of gas–liquid contactors such as bubble columns. For high-throughput processes such as processing of flue gas, low pressure drop is important to minimize the cost and energy required when pumping fluids through the column. Another issue that is important for the safety and reliability of the process is chemical compatibility of the materials coming into contact with the reactive fluids used in the process.

The ORNL team considered all the known characteristics that make an ideal absorber when investigating the performance of an absorption column equipped with commercial stainless-steel structured packing elements and a single PIPE device located near the middle of the column. The PIPE device not only provided high surface area for enhanced mass transfer, but it also allowed a cooling fluid to flow through the packing to remove the heat of the reaction without coming into direct contact with the reactive fluids. Because of its complexity, this novel aluminum PIPE was additively manufactured and required placement at a point along the column where the solvent reaches maximum (bulge) temperature for optimal CO_2 capture response. A 0.2 m diameter prototype of the PIPE is shown in Figure 1.

Figure 1. Additively manufactured PIPE for increasing CO_2 capture efficiency in solvent-based systems via integration of heat exchange functionality (Photo credit: C. Jones, ORNL).

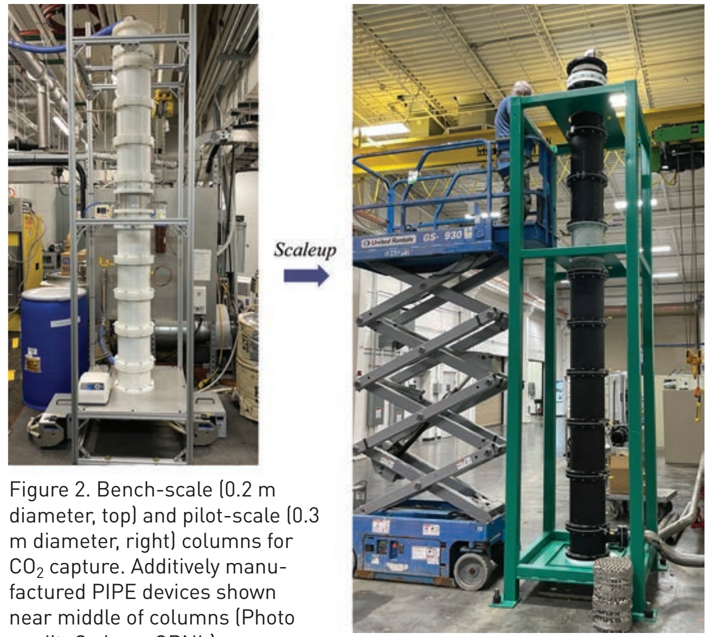

Figure 2. Bench-scale (0.2 m diameter, top) and pilot-scale (0.3 m diameter, right) columns for CO_2 capture. Additively manufactured PIPE devices shown near middle of columns (Photo credit: G. Jang, ORNL)

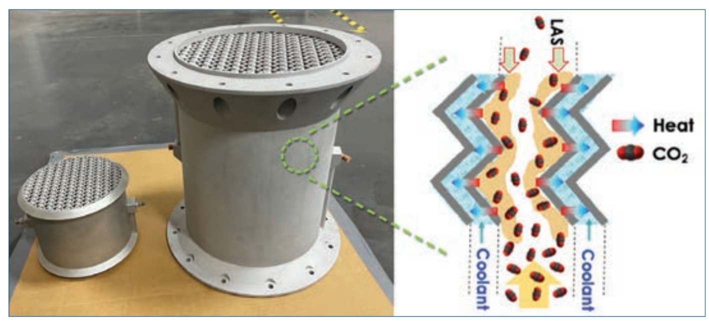

Figure 3. Left: scaleup of PIPE devices from 0.2 to 0.3 m diameter and from 0.17 to 0.41 m height via AM. Right: illustration of flow in PIPE device; cooling fluid flows within channels without contacting the reactive gas and solvent flowing in a countercurrent mode (Photo and schematic credit: G. Jang, ORNL).

RESULTS

The efficacy of the prototype ORNL-developed additively manufactured aluminum PIPE shown in Figure 1 was demonstrated in a bench-scale 0.2 m diameter column (Figure 2 left) for two different solvents, 30% by weight (~5 M) aqueous MEA and LAS, which were provided to the ORNL team by RTI International [12].

Solvent cooling achieved by the prototype PIPE was demonstrated to increase the CO_2 capture efficiency by as much as 15% using the aqueous MEA solvent and 25% using the LAS, which proved to be more temperature-sensitive compared to the MEA solvent. These encouraging results motivated scaleup of the absorber to a 0.3 m diameter (Figure 2 right) that can capture more than 1 tonne CO_2/day, scaling up by one order of magnitude compared to the 0.1 tonne CO_2/day that the 0.2 m column can capture.

Scaling up the absorber was made possible by scaling up the prototype PIPE device, as shown in Figure 3.

The pilot-scale column shown in Figure 2 (right) is in the final stages of commissioning and is being tested using nonreactive air–water fluids. It is expected to be available for CO_2 capture experiments in early 2023. The CO_2 source is a 100 kW natural gas–fueled generator with load and temperature control to produce realistic exhaust gas and load cycles representative of industrial operation. Because amine-based solvents have safe handling requirements, ORNL's Environmental Safety and Health team is engaged in the safe operation of the pilot-scale column.

CONCLUSIONS

ORNL has demonstrated additively manufactured process-intensification packing elements that can increase the CO_2 capture efficiency in gas–liquid absorption systems. A pilot-scale CO_2 absorber targeting capture of more than 1 tonne CO_2/day from realistic flue gas has been set up at ORNL for point-source capture research using a variety of solvents. The pilot-scale system is designed to be a flexible research platform to enable research of new solvents and various configurations of packing devices. Future work will focus on demonstrating intensified CO_2 capture using aqueous and low-aqueous solvents under realistic feed conditions.

IMPACT

AM enables realization of intelligent designs for packing structures for solvent-based CO_2 capture to enable process intensification, higher CO_2 capture efficiency, and potentially lower overall capital and operating costs for the point source CO_2 capture systems needed for power generation and industrial processes. In addition, the research provides critical data to investigate the effectiveness of various solvents for CO_2 capture, to validate predictive models that can subsequently be used for scaling up the process to the relevant industrial scale, and to develop control algorithms to manage transient conditions associated with load cycles in real-world operation.

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Additive Manufacturing of Radiation Detectors for Fundamental Science and National Security

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INTRODUCTION

Specially designed fluorescent plastics which emit light when exposed to ionizing radiation are used ubiquitously throughout the fields of medicine, fundamental physics, and national security. These inexpensive plastic scintillators can be used to detect many types of ionizing radiation, including X-rays, gamma rays, alpha and beta particles, and neutrons. Most contemporary plastic scintillators are formed through subtractive manufacturing (i.e., machining) methods in which large ingots are shaped into the desired forms. However, these approaches limit obtainable geometries, can generate significant plastic waste, and often lead to long production times. Additive manufacturing (AM) offers an attractive alternative manufacturing method that can produce near limitless geometries, reduce plastic wastes, and decrease production times. Geometries which would be difficult-to-impossible to produce using conventional methods can now be 3D printed. In collaboration with Lawrence Livermore National Laboratory and the Air Force Institute of Technology, ORNL is leading the development of light-based 3D printing of radiation detectors. Light-based vat polymerization techniques offer advantages for 3D printing of plastic scintillators, resulting in high optical clarity of 3D printed objects. Light-based 3D printing techniques require development of specialized resins that can be 3D printed as functional radiation detection materials with high spatial resolution. These newly developed 3D printed resins are being investigated for use in (1) the next generation of fast-neutron imaging systems for national security, and (2) fundamental science for future nuclear and high-energy physics experiments.

BACKGROUND

Although R&D of AM of radiation detection materials is in its early infancy, interest has been growing rapidly over the past few years. Radiation detection materials must posses and maintain their radiation detection properties after 3D printing. These properties include optical clarity, scintillation light yield, fast timing, and particle identification capabilities. Two main approaches are being considered for 3D printing of plastic scintillators: filament-based 3D printing, and light-based 3D printing. A filament-based 3D printing method known as fused deposition modeling (FDM) is a widely used AM method which builds up an object layer by layer through fusing of thermoplastic filament. 3D printing of radiation detectors by FDM has been demonstrated by several research teams [1–3]. FDM allows for multiple materials to be used to 3D print an object, making it possible to simultaneously 3D print an optically transparent radiation detector inside a reflective optical enclosure [2]. FDM printing of radiation detectors allows for traditional thermoplastic scintillator materials such as poly(styrene) and poly(vinyltoluene) to be used as-is with little or no modifications. The challenge is in the printing process itself. FDM printed objects often have significant optical defects such as voids between layers and rows of extruded filament which can scatter scintillation light. These effects can be reduced by carefully controlling the 3D printing parameters [2].

Light-based 3D printing techniques such as stereolithography (SLA) and digital light projection (DLP) rely on photopolymerization of liquid resin to create a 3D object layer by layer. In this process, liquid resin is housed within a vat with a transparent window in the bottom. A light source is projected onto the window in the shape of a cross-sectional slice of the 3D object being printed. This process is repeated until a fully 3D printed object is obtained. SLA and DLP differ by the way they project light onto the optically transparent window. SLA relies on a laser which rasters over the cross-sectional slice, and DLP uses a digital projector such as a liquid crystal display (LCD) screen to project the cross sectional slice. Light-based 3D printing of radiation detectors provides higher optical clarity and higher spatial resolution compared to FDM results. However, a completely new type of 3D printable radiation detecting resins is required for light-based 3D printing of radiation detectors.

Photopolymerization requires a significant departure from conventional thinking about how plastic scintillators are produced. Instead of using heat to induce polymerization, photopolymerization relies on light in a specific wavelength range to interact with compounds known as photoinitiators to induce polymerization. These photoinitiator compounds typically operate in the ultraviolet–to–low-visible wavelength range, with 405 nm being a typical light-based 3D printing wavelength. Because light-based 3D printing is a layer-by-layer process, it is desirable for photopolymerization reactions to be fast in order to reduce the total print time needed to create a 3D object. To date, several groups have demonstrated light-based 3D printable formulations which are functional radiation detection materials [4–6], but the overall performance of these formulations is below that of contemporary plastic scintillators.

RESULTS

High-performance photocurable resins. Traditional thermoplastic scintillator materials use poly(styrene) and poly(vinyltoluene) as a base material to which the fluorescent additives are added. The monomers (styrene and vinyltoluene) producing these polymers exhibit low reactivity under photopolymerization, making their use in light-based 3D printing impractical. To avoid this issue, a copolymerization method was developed which uses a blend of low reactivity monomers such as styrene and vinyltoluene with high reactivity, multifunctional monomers. The light output and particle discrimination capabilities of these 3D printed scintillators improves with higher poly(vinyltoluene) concentration. This improvement is the result of enhanced density of excitation and energy transfer with the higher poly(vinyltoluene) concentrations. Figure 1 shows four photocured scintillators with increasing poly(vinyltoluene) concentration. As the poly(vinyltoluene) concentration is increased, the clarity increases, and the unwanted discoloration decreases.

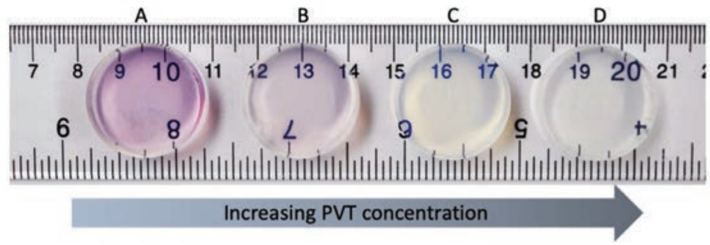

Figure 1. Photopolymerized scintillators as a function of poly(vinyltoluene) concentration. The increase in poly(vinyltoluene) improves the clarity, decreases discoloration, and improves radiation detection performance (Credit: M. Febbraro).

Improving 3D printing spatial resolution. AM makes it possible to produce geometries which would be difficult or impossible to produce using conventional methods. To do this efficiently, optimized resin chemistry and 3D printing equipment are required. With regards to resin chemistry, a number of resin parameters can affect the spatial resolution of a 3D printed object. These parameters include viscosity, cure time, and cure depth, which is the depth at the curing wavelength for which some fraction of light penetrates (i.e., 90% of light absorbed with some distance) into the resin or 3D printed object. The first two parameters can be controlled through the choice of the base resin. Control of the cure depth within a 3D printable radiation detector resin requires careful attention. Typically, the cure depth of a light-based 3D printing resin can be controlled by adding light-absorbing compounds which may or may not reemit light. Compounds which do not reemit light would significantly hinder radiation detection performance, so those are not selected. These compounds are commonly known as wavelength shifters. By design, scintillators are a cascade of wavelength shifters which efficiently convert high-energy depositions from ionizing radiation into relatively low-energy visible light. The concentrations of wavelength shifters are orders of magnitude more concentrated than that needed for cure depth control in light-based 3D printing. Because reducing the concentration of these wavelength shifters would deteriorate scintillator performance, an alternative approach was developed.

ORNL developed a new approach to decouple the radiation detection part of the resin chemistry from the 3D printing part. In this approach, the cascade of wavelength shifters needed for efficient radiation detection are designed to occur at a lower wavelength than that needed for 3D printing. The higher wavelengths are reserved for additives which optimize the spatial resolution of 3D printed objects. An example of a 3D printed object using this approach is shown in Figure 2. This decoupling scheme allows for separate, independent optimization of radiation detection and spatial resolution performance.

Figure 2. An evaluation print of "3DBenchy" demonstrating <100 um resolution under room (left) and UV (right) illumination. The bluish green glow shown in the right image corresponds to the same color glow emitted under exposure to ionizing radiation (Credit M. Febbraro).

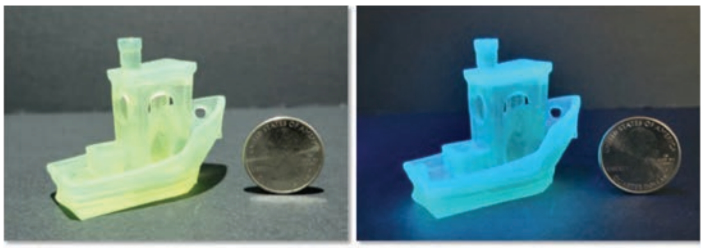

Figure 2. An evaluation print of "3DBenchy" demonstrating <100 um resolution under room (left) and UV (right) illumination. The bluish green glow shown in the right image corresponds to the same color glow emitted under exposure to ionizing radiation (Credit: M. Febbraro).

CONCLUSIONS

A new class of AM resins has been developed for light-based 3D printing of radiation detectors. A copolymerization technique has been developed to produce 3D printable resins that exhibit properties similar to those of traditionally manufactured materials. This allows good light yield and particle discrimination capability to be obtained in 3D printed objects. In addition, a new decoupling scheme demonstrates high 3D printing spatial resolution with radiation detection materials. The combination of these discoveries allows for high-performance plastic scintillators to be 3D printed with very good spatial resolution for detection of ionizing radiation.

IMPACT

The ability to additively manufacture radiation detection materials opens a wide range of new possibilities for fundamental science, national security, and beyond. This work has demonstrated that copolymerization and decoupling schemes can be implemented for 3D printing of high-performance plastic scintillators with very good light output, particle discrimination capability, and spatial resolution. These advancements enable new 3D geometries and applications which would be impossible to produce and perform using conventional subtractive manufacturing. Researchers are just scratching the surface of what is possible with AM of radiation detector materials, and the future looks promising.

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Advanced Materials Focus in 3D Printing and Advanced Characterization Suites at CNMS

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INTRODUCTION

Materials research advances are closely associated with ORNL. Beginning with the Manhattan Project during World War II, up through the current challenges posed by decarbonization, an all-encompassing approach to the science and technology of materials relies on strengths in computation, synthesis, and characterization. ORNL is also strong in manufacturing, with capabilities ranging from the manufacture of isotopes to advanced metal alloys. ORNL contributes significantly to solving challenges in energy generation, battery storage, decarbonization, and recycling. ORNL research facilitates the discovery and processability of materials by focusing on the dynamics, composition, structure, and scalability of new materials. ORNL ensures the availability of research tools and, more importantly, the expertise needed to orchestrate high-risk projects through the high-level skills of seasoned scientists and engineers. The COVID-19 pandemic resulted in ORNL's capabilities in advanced manufacturing being harnessed in a unique way [1,2].

BACKGROUND

Advanced materials have extensively engineered properties created through the development of specialized processing methods and synthesis technologies. Very often their development relies on knowledge of basic science platforms (fundamental discovery) and translation of those properties into high functionality or useful applications. The key is to understand structure-composition-processing-property relationships. This learning phase is followed by a focus on scalability in manufacturing. Advances using this approach have enhanced the introduction of advanced ceramics, high-value-added metals, electronic materials, composites, polymers, and biomaterials. Specifically, upcyclable polymers, high-entropy alloys, 2D nanomaterials composites, and energy storage materials have been prioritized because of the need to reduce the energy costs and carbon footprint of manufacturing. However, to ensure that these material advances benefit society, their manufacturability must be addressed.

Additive manufacturing (AM) enables new fabrication methods that result in high performance with more complex designs in parts [3]. AM, which is also known as *3D printing*, is essentially a layering or sintering process (Figure 1). Other more conventional methods are classified as *formative manufacturing* (FM), such as molding, casting, forming, injection molding, and as subtractive manufacturing (SM); the latter includes machining, milling, or cutting, which can generate more waste (Figure 1). AM has the advantage of enabling complex geometric designs that can be initiated as computer-aided designs and sliced (G-code optimization) to a host of layering or additive methods to build up the 3D structure. There are roughly three types of 3D printing technologies: sintering, melting, and stereolithography. These types include fused deposition modeling (FDM), binder jet, selective laser sintering (SLS), digital light projection, stereolithographic apparatus (SLA), and others. FDM, SLA, and digital light projection methods are used extensively to produce high-performance nanocomposites, thermoplastics, and thermosets [4]. For metal alloys, direct metal laser sintering, arch wire metal deposition, and indirect binder jetting of metal-containing resins are some of the options. Although each of these methods has inherent advantages over the others, each has been developed to take advantage of computer numerically controlled methods, or in the case of photocured processes, light projection from microlenses.

The advantages of AM compared with more conventional methods are as follows: (1) rapid prototyping and design optimization, (2) simplification and reduction of the number of parts for assembly, (3) limited production of the part or product for field applications, (4) remote or on-demand production, and (5) distributed production and reduction of inventory. All of these advantages can reduce time and cost for any given project. Industries heavily influenced by AM include automotive, aerospace, biomedical, oil and gas, and tooling industries,

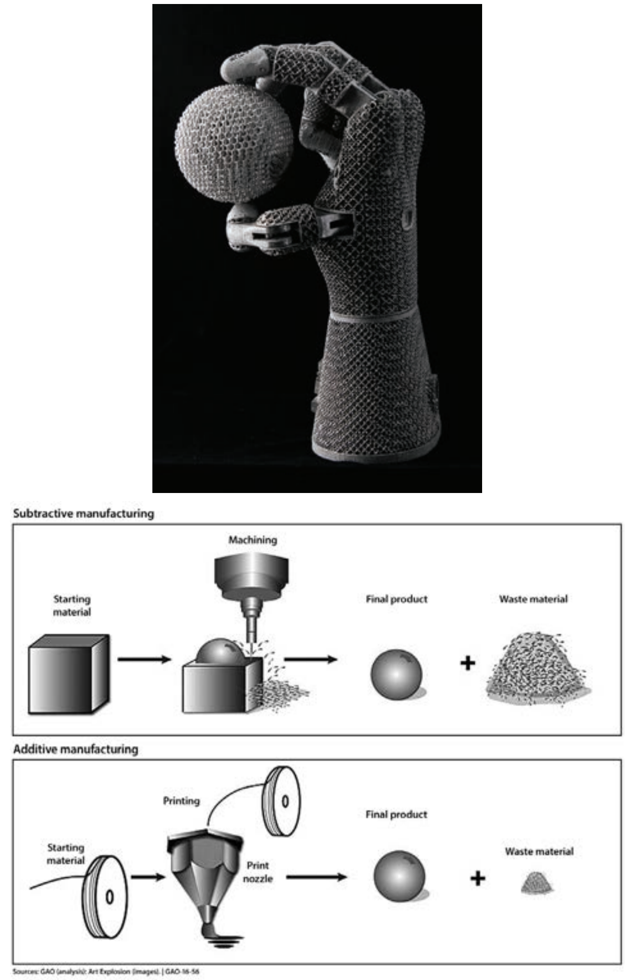

Figure 1. Top: lightweight, low-cost fluid powered robotic hand fabricated by electron-beam AM at ORNL (Credit: J. Richards, ORNL); bottom: conventional subtractive manufacturing and additive manufacturing. (Modified from US Govt. Accountability) [5].

as well as small-scale original equipment manufacturing, microelectronics, and construction. Combining AM, FM, and SM processes will truly make engineering design and testing capabilities occur at a rapid phase.

RESULTS

AM materials studies and CNMS. ORNL is home to the Manufacturing Demonstration Facility (MDF) [6] and the Carbon Fiber Technology Facility. As a world-renowned center of scalable AM technologies, MDF has many successful consortium industry partners. New manufacturing developments at MDF and the combination of FM and SM methods have propelled AM into more mainstream prototyping and manufacturing. The Center for Nanophase Materials Sciences (CNMS), a DOE Office of Science nanoscience research center and user facility [7], is also located at ORNL. ORNL also boasts several advanced neutron production and characterization facilities, such as the Spallation Neutron Source and the High Flux Isotope Reactor. Advanced materials studies are carried out at CNMS to gain understanding and control of electronic and molecular behavior at the nanoscale in a multidisciplinary, interdisciplinary setting.

As a user facility, CNMS allows users to take advantage of its advanced capabilities for characterization and materials studies using state-of-the-art equipment and methods for sample preparation, fabrication, and clean-room protocols.

In the field of materials and nanomaterials, important breakthroughs are realized through understanding phenomena and establishing basic science platforms from which new technologies can evolve. It is essential to have access to analytical tools such as spectroscopic, microscopic, and scattering capabilities that combine the state of the art with hyphenated and in-operando methods. This approach enables the time of observation to be matched with the corresponding resolution or frequency of the experiment or instrument. CNMS is well equipped to meet the challenges of AM characterization requirements with the appropriate empirical design and characterization methods down to the nanoscopic level.

AM material challenges. Specific AM materials include polymers such as thermoplastics, elastomers, and thermosets in the form of filaments, powders, viscoelastic materials, and curable liquid resins. Metal alloys are in the form of powders; wires that undergo melting or plasma heating; and blended resins, composites, and extrudable pastes that are later autoclaved to remove the polymer part. Ceramics can be in the form of powders, precursors of liquid resins, and extrudable pastes that can also be converted. Materials studies are required to optimize their processing conditions as "raw materials" for AM. Often their bulk properties are not the same as predicted at the nano- and micro-scale levels. Proper dispersion in host matrices or liquids is required, which is often associated with intractable phase behavior or poor surface/interface wetting in heterogeneous blends [8]. Thermal properties are complicated in highly formulated compositions because of differences in the enthalpic behavior of the components. Curing kinetics are complicated by the need to balance viscosity-thixotropic behavior and the availability of cross-linkable bonds. A number of these materials' properties must be optimized with the intended AM processing method.

It is important to address the many challenges presented by AM with a materials study and a real-time manufacturing adjustment or machine development approach. Challenges include (1) residual stresses caused by entrapment of nonequilibrium and metastable phases during processing, (2) poor adhesion between deposited layers, (3) entrapment of gases or evolved biproducts created during fabrication, (4) poorly matched thermal properties with the melt-quenching transitions, (5) incomplete curing kinetics matched with the layer build-up, and (6) lack of alloying and use of annealing or post-AM finishing procedures. Specific opportunities have been identified with the 3D printing of epoxy-polybenzoxazine-based shape-memory materials (Figure 2). Some of the 3D printed composites can be utilized for separation/filtration [9] and membrane enhancement for carbon capture [10]. The hierarchy of the materials' order and composition necessitates investigation on molecular, nanoscopic, microscopic, and macroscopic levels. The use of characterization tools that examine and correlate observed phenomena at these various levels makes it possible to define solutions that are often associated with a nonequilibrium processing environment.

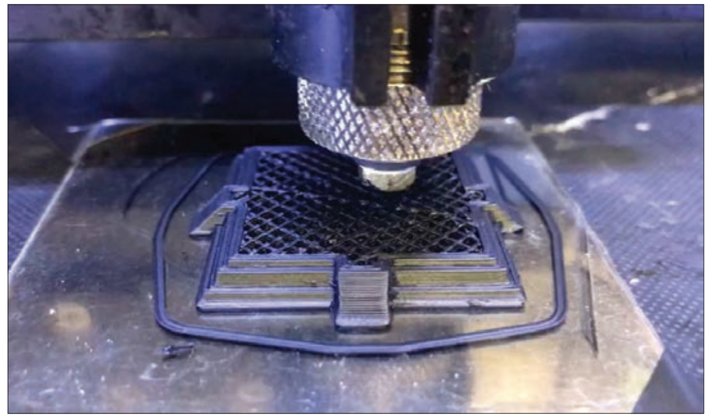

Figure 2. 3D printing of an epoxy-polybenzoxazine thermoset material. (Credit: R. Advincula).

Applications of AI/ML. The potential to use artificial intelligence (AI) and its subset of machine learning (ML) for statistical methods and deep learning (DL) in neural networks can optimize the 3D printing process and the testing protocols for fabricated parts (Figure 3) [11]. AI makes it possible to explore experiment design, Weibull optimization methods, and specific algorithms to improve the formulation composition of the materials and the parameters for 3D printing. In situ sensors can be designed as part of the 3D printer to provide a real-time feedback loop mechanism and data gathering so that the 3D printing process can be modified in real time. AI can improve the throughput of design iterations to arrive at the right balance of material properties with new geometric designs. AI can be used to achieve faster, more targeted testing methods to arrive at the property of interest for AM.

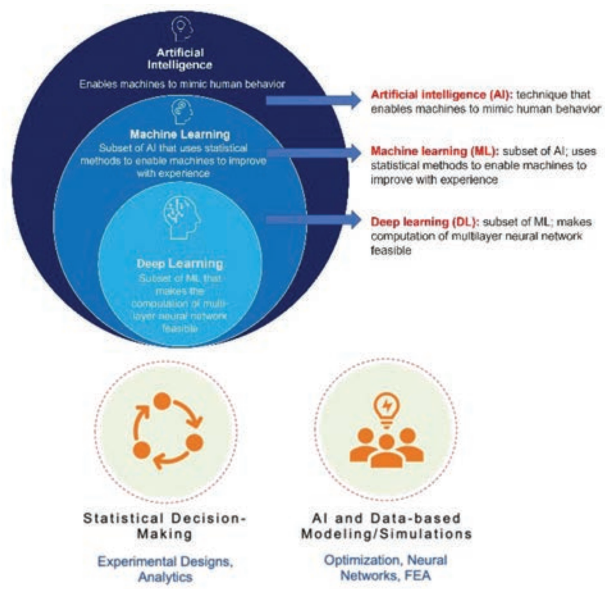

Figure 3. Needs for AI, ML for statistical methods, and DL in neural networks to optimize 3D printing. (Credit: R. Advincula).

CNMS Capabilities. CNMS can enable research capabilities in materials synthesis, characterization, simulation, and AI to contribute leadership in a comprehensive AM materials program at ORNL. These can accelerate the development of new materials and processing technologies to facilitate more rapid adoption by the AM community and the MDF. Users and collaborators can access state-of-the-art equipment in nanoscience and materials research, including synthesis, nanofabrication, spectroscopy, and imaging-microscopy. Modeling and simulation is one of the strongest capabilities at CNMS because the center has access to fast, world-leading computational capabilities at ORNL. Access can be obtained through peer-reviewed proposals. Because of the proximity of CNMS to the Spallation Neutron Source, the engagement also allows access to the wider nanoscience community.

Advanced characterization and fabrication methods at CNMS include thin film deposition and microscale synthesis, as well as processing of nanomaterials in hybrid architectures. These can be investigated in real time with operando spectroscopic characterization methods. Functional surface probe microscopy or atomic force microscopy (AFM) capabilities for materials at the nanoscale are enabled with in situ scanning probe imaging and spectroscopy techniques. Scanning tunneling microscopy can enable deep insight into the electronic, magnetic, and transport properties in low-dimensional systems and the behavior of quantum systems. Structure, chemistry, and function can be understood at the nanoscale level with atom probe tomography, in situ scanning transmission electron microscopy (TEM), and cryogenic electron microscopy techniques. Scanning transmission electron microscopy and scanning electron energy loss spectroscopy techniques provide spatial, temporal, and energy resolution limits for imaging and spectroscopy up to the nanoscale level. The analysis of cellulose nanocrystals or nanowhiskers by TEM and AFM is shown in Figure 4a. Nanofabrication capabilities are available for fabricating micro- and nanostructures with state-of-the-art lithography, thin-film deposition, ion-beam and e-beam etching, or cutting and

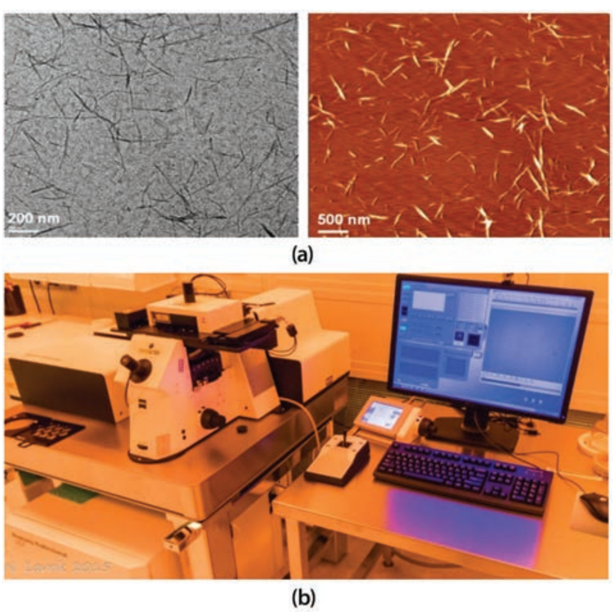

Figure 4. (a) TEM (left) and AFM (right) micrograph of cellulose nanowhiskers derived from coconut coir for SLA resin composites (Credit R. Advincula), and (b) Nanoscribe Photonics Professional GT stereolithography system for 3D micro- and nano-scale structures at CNMS (Credit: N. Lavrik, ORNL).

characterization tools in a clean room setting. The center is also host to nanoscale 3D printing instrumentation (Nanoscribe-2) via 2-photon polymerization (Figure 4b).

In a number of these characterization and synthesis/processing methods, edge computing and AI/ML methods can be used to accelerate discovery [12]. Through the Nanomaterials Theory Institute, it is possible to access capabilities for theory and high-performance simulation ranging from atomistic to coarse-grain levels to predict the physical and chemical properties of materials and soft matter through simulation and theory.

Polymer materials for AM. The strong suite for polymer synthesis and characterization by the macromolecular nanomaterials group at CNMS is a natural partner for polymer-based AM materials. The group is capable of precision synthesis of functional polymers to create thermoplastics, thermosets, and elastomers. It supports selective deuteration (for neutron studies), small molecule synthesis, and ionic polymerization, as well as several macromolecular characterizations such as gel permeation chromatography, light scattering, thermal analysis, and nuclear magnetic resonance spectroscopy. Two new CNMS facilities built over the past three years specifically benefit the AM community. A 3D printing laboratory is equipped with state-of-the-art machines for FDM, SLS, SLA, direct ink writing, and filament fabrication/recycling. The new capability for scalable polymer manufacturing is the continuous flow chemistry and polymerization reactors equipped with online sensing instrumentation (nuclear magnetic resonance, gel permeation chromatography, infrared) and a feedback-loop control that will be enabled by AI [13]. This is part of ORNL's INTERSECT initiative.

Specific projects that can take advantage of the new 3D printing capabilities and scalable synthesis at CNMS are related to (1) 3D printing and stability of polyelectrolyte complex coacervates, (2) continuous fiber epoxy composites and the enhancement of interfacial adhesive behavior, (3) 3D printing of cementitious carbon-capture materials, (4) in situ investigation of nonequilibrium properties in thermoplastics and thermoset 3D printing, (5) investigation of phase migration and kinetics of adhesion promoters in FDM 3D printing, (6) investigation of surface properties of micronized powders and mixed-grain methods for SLS and direct metal laser sintering 3D printing, (7) 3D printing of battery electrode materials, (8) 3D printing of recycled and upcycled polymer materials, and (9) 3D printing of membrane and separation materials [9,10].

During the initial stages of the COVID-19 pandemic emergency, ORNL demonstrated the potential of AM and advanced prototyping and manufacturing by (1) MDF's distributed manufacturing of face masks through rapid prototyping and deployment using AM [1,2], (2) the Carbon Fiber Technology Facility's development of effective filtration media and respirator technology (N95) against airborne viruses such as COVID-19 [14], and (3) CNMS's development of a rapid testing device for collecting pathogens and sampling them [15] (Figure 5). AM methods and the capability to rapidly prototype with materials and design were crucial in meeting national emergency needs.

CONCLUSIONS AND IMPACT

Efforts to develop advanced materials and to serve the broad needs of the AM community can take advantage of both the

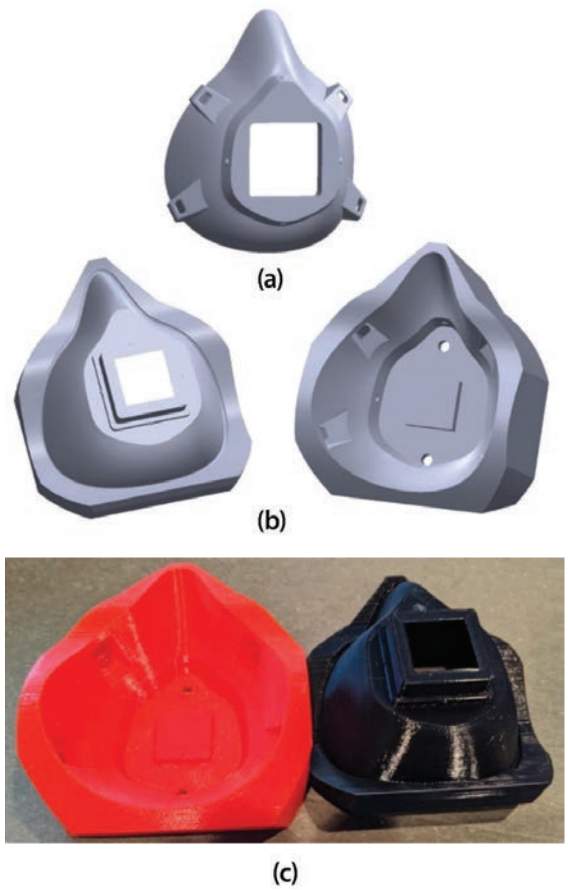

Figure 5. 3D printing of a mask prototype for distributed AM manufacturing showing (a) injection molded thermoplastic mask frame, (b) computer-aided design of the mold that can be made from high-performance composite or metal alloy based on 3D printing, and (c) actual 3D printed female (left) and male (right) mold halves (Credit: A. Roschli) [1].

capabilities and expertise of MDF and access to user facilities such as CNMS. The CNMS is renowned for enabling new basic science platforms and fundamental discovery among its users, and it is poised to help translate those properties into high functionality or useful applications, especially through a greater understanding of the structure-composition-processing-property relationship. AM enables new fabrication and rapid prototyping and optimization. However, there is a need to understand and control a hierarchy of raw materials properties, from nanoscopic to macroscopic, to optimize the fabrication process and to enable high performance for their intended applications. Important capabilities for spectroscopic analysis, microscopic characterization, sample preparation, scale-up synthesis, fabrication, and clean room protocols are key to advancing knowledge of advanced materials and processing for AM. A highlight of AM in advanced prototyping and characterization was demonstrated in the recent response to emergency needs created by the COVID-19 pandemic.

COLLABORATE WITH ME

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