OAK RIDGE NATIONAL LABORATORY

Review

Preparing for disaster:

OAK RIDGE National Laboratory

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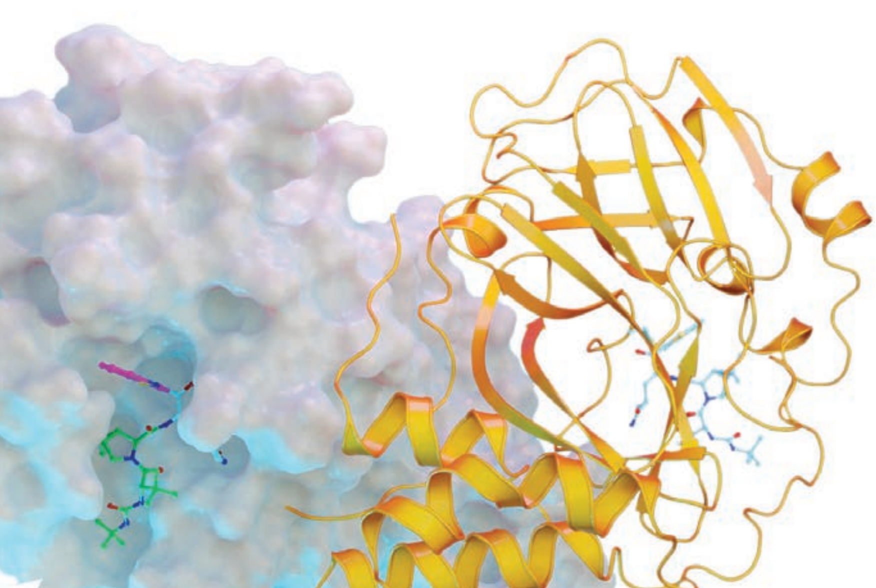


On the Cover

Supriya Chinthavali leads the lab's Geoinformatics Engineering Group.
Image credit: Carlos Jones, ORNL

National security for the 21st century

Oak Ridge National Laboratory was created to solve a national security challenge — specifically to harness the power of the atom before America's World War II adversaries.

That was 1943. At the time, there was no internet and, hence, no cybersecurity threat. Nor was climate change a major concern, with its accompanying heat waves, droughts and severe weather.

Needless to say, threats to our national security have evolved significantly in the nearly eight decades since ORNL began. Nuclear nonproliferation is still a priority, but many other challenges have emerged.

In the new national security landscape, researchers in fields ranging from high-performance computing and artificial intelligence to climate science must collaborate to apply their specialties to complex threats.

This is where national laboratories excel. ORNL has been a center of nuclear science and technology since its inception, and as DOE's largest science and energy laboratory today, we are a powerhouse in materials, isotopes, neutron science, computing, advanced manufacturing and energy technologies.

In this issue of *ORNL Review*, we take a close-up look at the national security challenges being addressed by the talented researchers and scientific tools available at ORNL (See "National security science tackles a new generation of threats," page 8).

For example, ORNL supports the nation's nonproliferation work both with people (see "Engineers and scientists support nonproliferation efforts," page 24) and with state-of-the-art equipment (see "High-performance computing boosts uranium research," page 14).

Computing is also a powerful tool informing disaster response, where it is combined with ORNL expertise in geospatial science (see "ORNL tools help ensure energy supply," page 16).

In addition, ORNL researchers are helping energy utilities keep power flowing by providing guidance both on choosing cybersecurity tools and on evaluating existing products that may contain bugs, counterfeit parts or undocumented functionality (see "Strengthening cybersecurity in the energy sector," page 20).

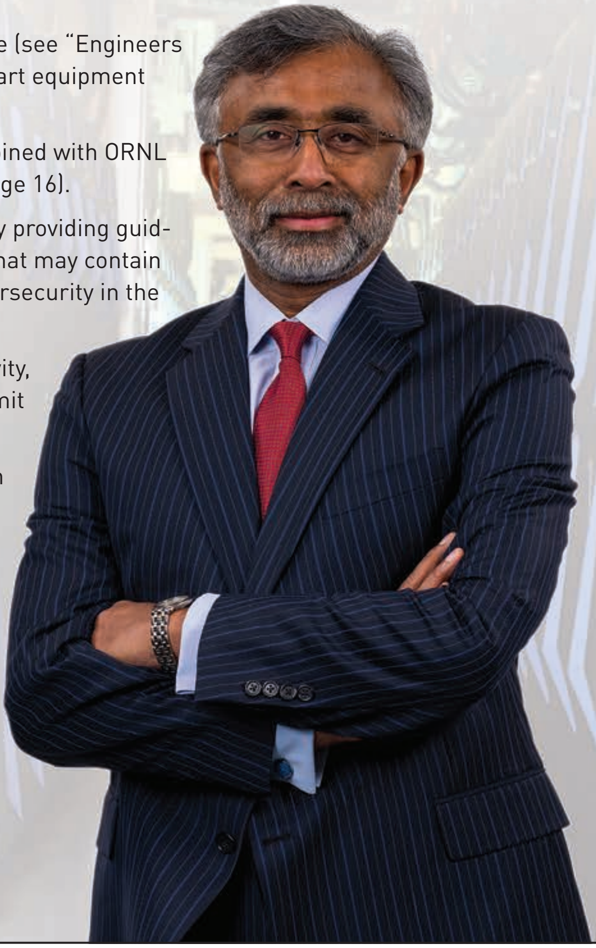
Elsewhere in this issue of *ORNL Review*, we look at research into superconductivity, or the ability of a material to conduct electricity with zero resistance (see "Summit study tackles superconductivity," page 26).

We discuss the work of an ORNL team that used scanning transmission electron microscopy to machine nanoscale cubes and place them in arrangements that could lead to faster computer chips and more powerful sensors (see "Precision machining produces tiny, light-guiding cubes for advancing info tech," page 36).

We look at a project that engineered microorganisms that turn industrial emissions into acetone and isopropanol, chemicals that serve as the basis for thousands of products (see "Microbes turn waste gases into valuable chemicals," page 40).

Finally, in the third edition of our *Research Insights* section, our technical staff highlight advances they have made to help the country reduce greenhouse gas emissions.

I hope you enjoy learning about contributions ORNL is making in national security, climate, and across our research portfolio in this issue of *ORNL Review*.



Thomas Zacharia
Laboratory Director

ORNL Director Zacharia announces retirement

Thomas Zacharia has announced his intent to retire as director of Oak Ridge National Laboratory at the end of 2022, the culmination of a 35-year career at the nation's largest science and energy laboratory.

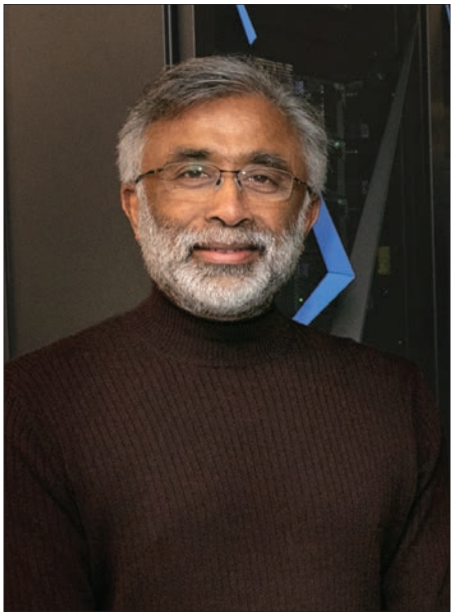
Zacharia has served as laboratory director since July 2017, overseeing the lab's extensive $2.5 billion research portfolio and staff of nearly 6,000.

"An incredible leader, extraordinary collaborator and powerhouse innovator, Thomas is leaving a profound impact on ORNL and the world," said Randy Boyd, University of Tennessee system president and chairman of the UT-Battelle Board of Governors. UT-Battelle operates ORNL for DOE's Office of Science.

In his tenure as laboratory director, Zacharia spearheaded significant growth in ORNL's staff and portfolio, established new research initiatives, and guided the lab through the COVID-19 pandemic.

Among milestones in Zacharia's tenure as director, the laboratory has:

- continued deployment of a series of world-leading supercomputers; the latest, Frontier, broke the exascale barrier with a speed in excess of a quintillion calculations per second and premiered at No. 1 on the world TOP500 list in May;
- advanced world-leading neutron research through the Proton Power Upgrade at the Spallation Neutron Source and launched the Second Target Station project;
- established and led critical multi-institutional research efforts, including the Exascale Computing Project, Quantum Science Center and Center for BioEnergy Innovation;
- partnered with the University of Tennessee to establish the UT-Oak Ridge Innovation Institute to help develop the industries and workforce of the future.



Thomas Zacharia

- led U.S. contributions to the international ITER project and launched the Materials Plasma Exposure Experiment to support the development of fusion energy;
- invested in isotope research and production capabilities, including the Stable Isotope Production Facility and Stable Isotope Production and Research Center;
- focused attention on the application of science to national security challenges with creation of a new National Security Sciences Directorate; and
- assembled the most diverse leadership team ever at the lab.

"I am very optimistic about ORNL's future and in its pursuit of excellence — to be among the premier research institutions in the world," Zacharia said in a message to staff members. "I am very proud that mission and service continue to define ORNL on the eve of its 80th anniversary. We are stewards of an amazing legacy, and there comes a time when we all must pass that responsibility along."

Zacharia joined ORNL in 1987 as a postdoctoral researcher and rose through a series of leadership positions in computing, including establishment of the Computing and Computational Sciences Directorate in 2001. — *Morgan McCorkle*

Proteins linked to cancer, paving the way for therapies

ORNL researchers have definitively linked the function of a specific domain of proteins important in plant–microbe biology to a cancer trigger in humans — knowledge that had eluded scientists for decades.

The team's findings, published in *Nature Communications Biology*, open up a new avenue for the development of drug therapies to fight a variety of cancers, such as those that begin in the breast and stomach.

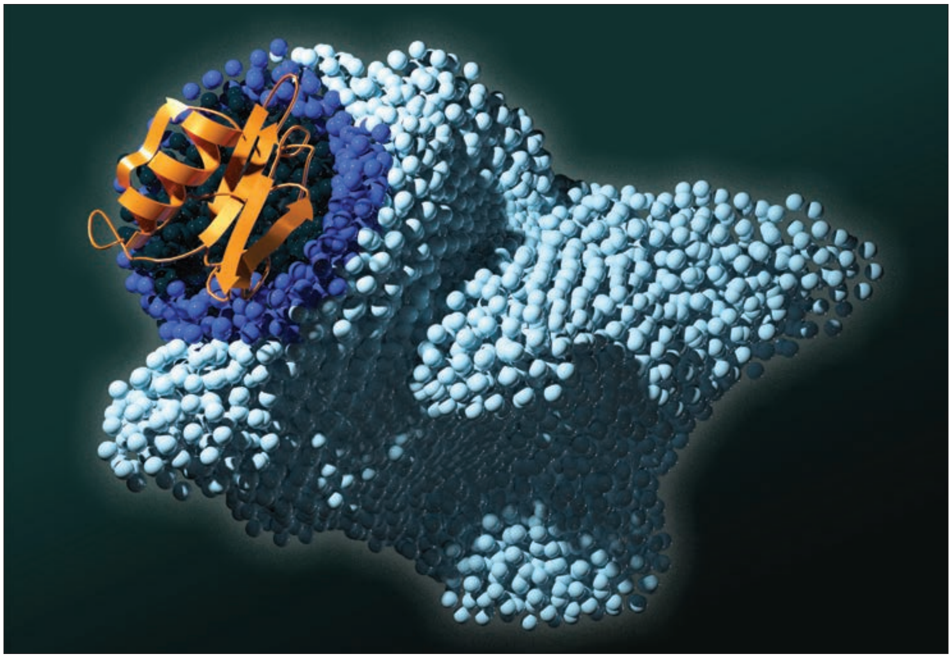
The scientists set out to prove experimentally what they first deduced with computational studies: that the plasminogen-apple-nematode, or PAN, domain is linked to the cell proliferation that drives tumor growth in humans and defense signaling during plant–microbe interactions in bioenergy crops. The association was first made as researchers explored the genomes of crops such as poplar and willow.

In the latest study, the ORNL team pinpointed four core amino acids called cysteine residues in the Hepatocyte Growth Factor, or HGF, a protein that is critical to the PAN domain's function, and studied their behavior in human cancer cell lines. They found that mutating any one of those amino acids turned off a signaling pathway known as HGF-c-MET. That pathway is abnormally heightened in cancer cells, causing them to rapidly multiply and spread.

Because cysteine residues are known to have many functions, the scientists also randomly tested other cysteines throughout the protein and found that none of them had the same impact on HGF-c-MET signaling. Mutating the four key cysteines had no effect on the overall structure of the protein and merely inhibited the cancer signaling pathway.

Disrupting the right signal is one of the biggest challenges in developing new cancer therapies, said ORNL geneticist Wellington Muchero.

"It's very difficult to engineer molecules to interfere with an entire protein," he said. "Knowing the specific amino acids to target within that protein is a big advancement.



ORNL scientists identified four amino acids key to signaling pathways in the PAN protein domain. Mutating any of those four resulted in disruption of the signal that tells cancer cells to multiply and spread in humans. Image credit: Andy Sproles, ORNL

You don't have to search the entire protein; just look for these four specific residues." — *Stephanie Seay*

For more information: https://bit.ly/3af8Gks

Report looks to dams as untapped power sources

Although there are more than 92,000 dams across the country, the vast majority — about 89,000 — do not generate electricity through hydropower.

ORNL researchers are assessing the viability of retrofitting some of these nonpowered dams, which may add up to 12 gigawatts of additional electricity to the power grid — enough to power 9 million homes, or every home in Tennessee, Alabama and Georgia.

In a new report released by the DOE, ORNL identifies key development challenges, including aging infrastructure, dam design limitations, costs, timelines and environmental considerations. The goal is to accelerate design approaches and innovations that increase energy from hydropower while ensuring environmental compatibility and economic feasibility.

"Hydropower has over 100 years of history in the U.S.," said ORNL's Scott DeNeale. "DOE's continued investments position the industry well to power untapped water infrastructure while achieving low-impact renewable energy growth." — *Mimi McHale*

Study shows that bacteria help peat beat the heat

Microorganisms may provide hope that peatlands can withstand hotter temperatures in a changing climate.

ORNL scientists have discovered that certain bacteria increase the climate resilience of *Sphagnum* moss, the tiny plant responsible for storing a third of the world's soil carbon in peat bogs. Heat-tolerant microbes transfer that protection to the plants, helping them survive climate warming.

A better understanding of the mutually beneficial partnership, or symbiosis, between moss and microbes could point to new paths for maintaining healthy moss and preserving these vital peatland ecosystems.

"Perhaps everything isn't as dire as we think," said ORNL's David Weston, a plant biologist and lead of the recent study. "Maybe organisms are more resilient than we know to these extreme climatic conditions. We're seeing that you can drastically influence an organism's ability to handle these stressful conditions just on its associated microbiome."

The research team found that hotter temperatures change the composition

Nonpowered dams such as Byrd Creek Dam in Crossville, Tennessee, may prove viable as retrofitted hydropower facilities. Image credit: Scott DeNeale, ORNL

Sphagnum *moss is the tiny plant responsible for storing a third of the world's soil carbon in peat bogs.*
Image credit: Genevieve Martin, ORNL

of the microbial communities, or microbiomes, living in *Sphagnum* moss. This change in community composition causes the moss to activate certain genes that trigger the production of hormones and proteins known to confer stress tolerance.

The team demonstrated that heat-tolerant microbes, when applied to laboratory moss grown without a microbiome of its own, elicit the same protective response and enable moss to better survive heat waves.

The findings offer a glimmer of hope for the moss and its function in sequestering carbon as temperatures increase. Previous ORNL study results have shown that sections of warmed peat bog in a whole-ecosystem manipulation experiment changed from carbon accumulators into carbon emitters in just three years, releasing carbon dioxide and methane into the atmosphere. — *Kim Askey*

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

ORNL's Ozpineci selected for Nagamori Award

Burak Ozpineci, a Corporate Fellow and Vehicle and Mobility Systems section head at ORNL, is one of six international recipients of the eighth Nagamori Award, chosen annually by the Nagamori Foundation based in Kyoto, Japan. The honor recognizes outstanding researchers and engineers working in electric motors, motor drives and related fields.

At ORNL, Ozpineci's research focuses on electric drive technologies and wireless charging. He was recognized for his research developing low-cost, high-efficiency, compact electric motor drives for electrified transportation systems.

"I am honored to be recognized by the Nagamori Foundation," Ozpineci said. "It's a privilege to be one of the researchers chosen for this prestigious award highlighting my contributions to transportation electrification through my 20-plus year career."

Burak Ozpineci

In addition to the Nagamori honor, Ozpineci was named a fellow of the Institute of Electrical and Electronics Engineers for contributions to transportation electrification and wireless charging of electric vehicles. The IEEE Power Electronics Society recognized Ozpineci with the IEEE PELS Vehicle and Transportation Systems Achievement Award. He has earned several Distinguished Achievement awards from DOE, holds two R&D 100 awards and co-leads DOE's Electric Drive Technologies Consortium.

"Burak is a recognized leader in power electronics research, and he is well known for his scientific achievements in wireless charging," said Robert Wagner, director of ORNL's Buildings and Transportation Science Division. "He's also a true innovator, whose pioneering work has advanced our understanding of vehicle power electronics. I am pleased to see him receive this international honor from the Nagamori Foundation." — *Jennifer Burke*

ORNL sponsors cohort of Black entrepreneurs

ORNL is sponsoring a cohort of 100Knoxville, a five-week mentorship and support program for Black founders of businesses.

"We're honored to support Black entrepreneurs through 100Knoxville," said ORNL Director Thomas Zacharia. "I look forward to seeing how ORNL's investment in the cohort's businesses contributes to a stronger and more diverse Oak Ridge Corridor."

The goal of 100Knoxville, a Knoxville Entrepreneur Center program, is to help Black-owned businesses grow through a focused investment of time and talent, while also providing access to social, political and financial capital. Each of the five entrepreneurs in a cohort is paired with a team of mentors for five weeks to clarify strategy, improve operations and, most importantly, increase sales. Each firm will receive $5,000 to invest at the direction of the entrepreneur with the support of their mentors.

Jade Adams, owner of the popular Knoxville plant boutique Oglewood Avenue, was a member of the first cohort of 100Knoxville. ORNL is sponsoring the sixth cohort of the mentorship and support program for Black founders of businesses. Image credit: 100Knoxville/Knoxville Entrepreneur Center

"ORNL's success is connected to the growth of the entrepreneurial ecosystem in East Tennessee," said Susan Hubbard, deputy for science and technology at ORNL. "We're supporting 100Knoxville because we understand how access to expertise and mentorship can help new businesses and entrepreneurs flourish."

In her role at ORNL, Hubbard oversees the lab's partnerships in technology transfer, economic development and sponsored research.

The program's spring 2022 cohort, 100Knoxville's fourth, recently concluded. The fall cohort will begin in September. The ORNL-sponsored cohort will follow sometime after. Each cohort is facilitated by strategist and business consultant Kandis Troutman, founder of the Creative Architect. — *Karen Dunlap*

Plastic upcycling improves feedstock for 3D printing

ORNL researchers have developed an upcycling approach that adds value to discarded plastics for reuse in additive manufacturing, or 3D printing. The readily adoptable, scalable method introduces a closed-loop strategy that could reduce plastic waste and cut carbon emissions tied to plastic production.

Results published in *Science Advances* detail the simple process for upcycling a commodity plastic into a more robust material compatible with industrial 3D-printing methods.

The team upgraded acrylonitrile butadiene styrene, or ABS, a popular thermoplastic found in everyday objects ranging from auto parts to tennis balls to LEGO blocks. ABS is a popular feedstock for fused filament fabrication, or FFF, one of the most widely used 3D-printing methods. The upcycled version boasts enhanced strength, toughness and chemical resistance, making it attractive for FFF to meet new and higher performance applications not achievable with standard ABS.

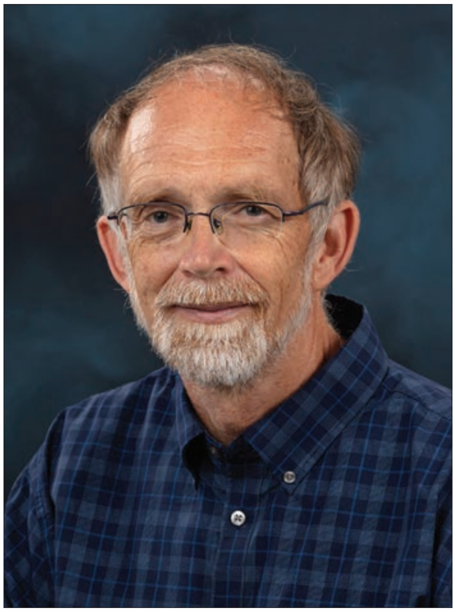
Polymer upcycling plays an important role in addressing the growing challenge of plastic waste accumulation. Approximately 400 million tons of plastic waste is generated each year, largely as single-use items that end up in landfills or the environment. Globally, less than 10 percent of plastic waste is recycled.

"We will need fundamental discoveries to overcome the challenges of increased costs and deteriorating material properties associated with recycling," said lead author Tomonori Saito of ORNL's Chemical Sciences Division. "Our goal was to develop an easily adoptable strategy that reuses plastic waste to create a more valuable material instead of generating fresh plastic."

The team targeted additive manufacturing, which is more resource efficient than conventional manufacturing and can achieve useful and complex 3D structures that would be difficult to produce by molding or casting. FFF makes up the largest share of this industry at nearly 70 percent of the global market. — *Ashley Huff*

For more information:
https://bit.ly/3AT5PID

ORNL polymer scientists Tomonori Saito, left, and Sungjin Kim upcycled waste plastic to create a stronger, tougher, solvent-resistant material for new additive manufacturing applications.
Image credit: Genevieve Martin, ORNL



Bobby Sumpter

ORNL's Sumpter elected fellow of two societies

Bobby Sumpter, an ORNL Corporate Fellow and Theory and Computation section head in the Center for Nanophase Materials Sciences, has been named fellow of two scientific professional societies: the Institute of Physics and the International Association of Advanced Materials.

"I am delighted to be named a fellow of these professional organizations," Sumpter said. "It presents a great opportunity to promote physics and materials science internationally."

Sumpter completed an undergraduate degree in chemistry from Southwestern Oklahoma State University and a doctorate in physical chemistry from Oklahoma State University. After completing postdoctoral work in chemical physics at Cornell University, he joined ORNL in 1988 as a postdoctoral research associate through the University of Tennessee, where he was studying polymer physics and chemistry.

In his more than 30 years at ORNL, Sumpter has held a variety of research and leadership positions.

Sumpter's Theory and Computation section includes the Nanomaterials Theory Institute and the Data NanoAnalytics Group. His work focuses on the development and application of modern computational and mathematical simulations to understand and predict complex behavior of materials ranging in scale from molecular to the nanoscale.

He is also a joint faculty member at the Bredesen Center for Interdisciplinary Research and Graduate Education, a UT–ORNL partnership.

IOP has recognized Sumpter for his "outstanding accomplishments in physics and his impact to materials and nanoscience including leadership, inspiration, opportunity and recognition." IAAM cited Sumpter "in recognition for contributions towards advancement of materials to global excellence." — *Sara Shoemaker*

New facility produces cosmic isotopes on Earth

Two decades in the making, a new flagship facility for nuclear physics has opened, and ORNL scientists have a hand in 10 of its first 34 experiments.

The Facility for Rare Isotope Beams, or FRIB, a DOE Office of Science user facility at Michigan State University, will produce more than 1,000 new rare isotopes.

These isotopes have abnormal proton-to-neutron ratios, so they are unstable and prone to decay. Many exist for mere fractions of a second. Until now, isotopes such as magnesium-40, calcium-55 and nickel-78 were made only in stellar explosions and neutron star mergers. Now, what is designed to be the world's most powerful heavy-ion accelerator makes them here on Earth.

"FRIB will launch a new era of discovery," said Witold Nazarewicz, a former ORNL Corporate Fellow who is FRIB's chief scientist and a distinguished professor of physics at Michigan State. "ORNL has provided long-term expertise and unique instrumentation that will help FRIB deliver new knowledge about what holds atomic nuclei together, how elements are created and how to use nuclei for societal benefits."

FRIB's first experiment is led by Heather Crawford of DOE's Lawrence Berkeley National Laboratory with partners at ORNL, the University of Tennessee, Knoxville, and elsewhere. The experiment employs the FRIB Decay Station initiator, or FDSi, a modular, multidetector system

ORNL's Mitch Allmond works with the Facility for Rare Isotope Beams Decay Station initiator, which combined diverse detectors for FRIB's first experiment. Image credit: Robert Grzywacz, ORNL that is extremely sensitive to rare isotope decay signatures.

"The FDSi is an assembly of the best detectors available in the scientific community within an integrated infrastructure for FRIB nuclear decay studies," said ORNL's Mitch Allmond, who manages the project. A key component of the FDSi originated from seminal work on germanium detector design by ORNL's David Radford, including the CLover Array for Radioactive ION Beams, or CLARION. — *Dawn Levy*

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

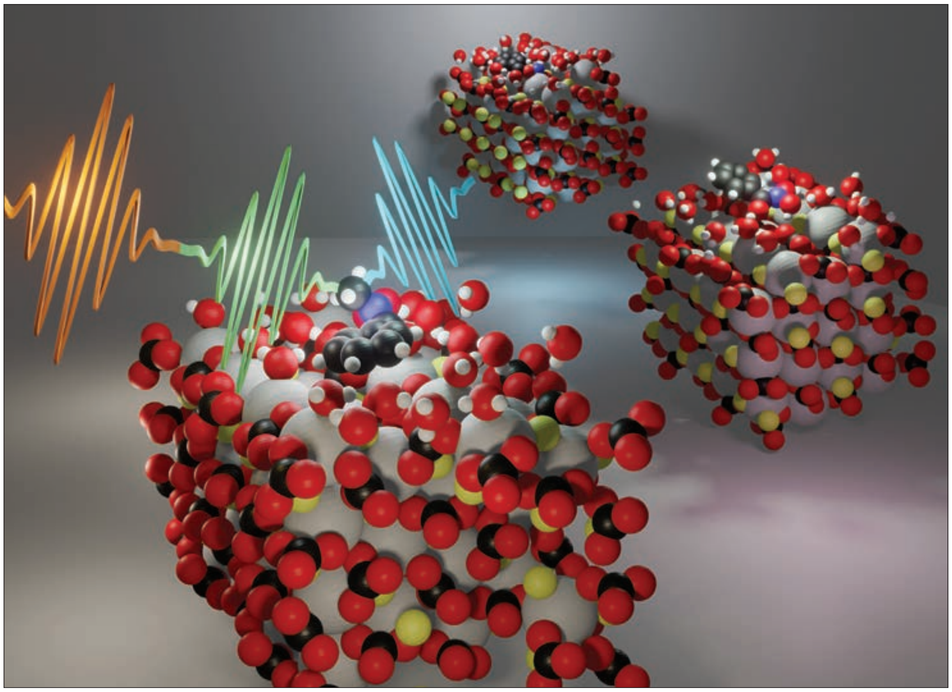
Materials tech focuses on chemical separations

ORNL researchers are using state-of-the-art methods to shed light on the chemical separations needed to recover rare-earth elements and secure critical materials for clean energy technologies.

Bastnäsite deposits in the United States are rich in rare-earth metals but must be mined and separated from unwanted minerals through chemical processes that are not well understood. Fundamental insights are needed to improve current recovery approaches, which are based largely on trial and error. Greater efficiency offers cost savings as well as benefits to the environment by decreasing mining and carbon impacts.

"The path forward will require predictive modeling to help us discover the best candidates for more efficient separations," said ORNL's Vyacheslav Bryantsev.

The team combined theory and spectroscopy methods to design collector molecules that buoy bastnäsite out of an ore mixture to enhance recovery by froth flotation. Their study supplies missing information for modeling future collectors tailor-made for efficient separations. — *Ashley Huff*



ORNL researchers shed light on chemical separations to recover rare-earth elements.
Image credit: Ben Doughty, ORNL

ORNL's Kothe to lead computing directorate

ORNL's Doug Kothe has been named associate laboratory director for the Computing and Computational Sciences Directorate, replacing the retiring Jeff Nichols.

Doug Kothe

"It's truly an honor and a privilege. I can't think of a better job to have and a better place to have it," Kothe said. "I'm really excited to join the best computing organization in the world, and CCSD is the best thanks to Jeff Nichols, who has had an incredible run in leading the directorate with vision, passion and commitment to be the best."

Kothe has led the Exascale Computing Project since 2017 and has more than 37 years of experience working in DOE national laboratories. He joined ORNL in 2006 as director of science for CCSD's National Center for Computational Sciences. From 2010 to 2015, Kothe directed the Consortium for Advanced Simulation of Light Water Reactors, DOE's first Energy Innovation Hub.

Prior to joining ORNL, Kothe spent 20 years at Los Alamos National Laboratory. He holds a bachelor's degree in chemical engineering from the University of Missouri, Columbia, and master's and doctoral degrees in nuclear engineering from Purdue University.

The Computing and Computational Sciences Directorate houses the Oak Ridge Leadership Computing Facility, a DOE Office of Science user facility that is home to Frontier, the world's fastest supercomputer. — *Morgan McCorkle*

National security science tackles a new generation of threats

by Eric Swanson
swansonej@ornl.gov

For centuries, national security was a face-to-face concern, with contests playing out in fields and oceans around the world. It was a battle of military might: Who had the larger army? Who could build the most powerful weapon?

But more and more, the battle has shifted. As the world has grown more technologically advanced and interconnected, the physical limitations of adversarial engagements have diminished.

> *"Most sciences are doing battle with natural laws, trying to understand or overcome the physical limitations of the natural world. When you get into national security science, you're looking at a challenge that's very different — you're dealing with adversaries, and our adversaries are very intelligent and dynamic.*
>
> — ORNL Cyber Resilience and Intelligence Division Director **Shaun Gleason**

"Science and technology are becoming more and more integral to national security," said Chuck Durant, director of Oak Ridge's Field Intelligence Element. "The adversary keeps evolving. The technology keeps evolving. We need to keep up our own research and intelligence capabilities."

Today, the battlefield is limitless and, often, invisible. Combating these evolving threats requires a scientific approach to national security.

"Most sciences are doing battle with natural laws, trying to understand or overcome the physical limitations of the natural world," said Shaun Gleason, director of ORNL's Cyber Resilience and Intelligence Division. "When you get into national security science, you're looking at a challenge that's very different — you're dealing with adversaries, and our adversaries are very intelligent and dynamic."

Recognizing this shift, ORNL established a National Security Sciences Directorate in 2018. It is structured largely around cybersecurity, nuclear security, human security and intelligence support, but as Associate Laboratory Director for National Security Sciences Moe Khaleel notes, solving today's challenges requires more than any single scientific discipline.

"The interesting thing about national security sciences is that to solve a national security challenge, you have to bring different areas of science together," Khaleel said. "And frankly, it's not just science; it's actually science, technology and analytical tradecraft — being able to use the tools of science to understand and communicate what our adversaries are doing."

Developing the science and technology required to advance national security missions is something ORNL has done since it was created during World War II's Manhattan Project (see "Engineers and scientists support nonproliferation efforts," page 24.)

"The entire existence of Oak Ridge came from a national security interest," said Budhu Bhaduri, director of the lab's Geospatial Science and Human Security Division. "Nuclear science is something that, in the past, we have invested in because of our national security interest."

Today, ORNL researchers are continuing the site's Manhattan Project legacy and advancing the science of nuclear nonproliferation. But they are also looking at emerging threats, such as cyberattacks on critical infrastructure and the national security implications of climate change.

See NATIONAL SECURITY SCIENCE TACKLES A NEW, page 10

In the Nuclear Nonproliferation Division, researchers like ORNL's Tyler Spano are delivering science-based solutions to reduce the risk that nuclear materials will end up in the wrong hands while enabling their secure use for peaceful applications across the world. Image credit: Carlos Jones, ORNL

NATIONAL SECURITY SCIENCE TACKLES A NEW, page 8

Reducing nuclear risks

Cary Crawford started his career in the nuclear industry at exactly the wrong time.

He joined DOE's Pantex nuclear weapons plant in 1993 — right when the new, post-Cold War order resulted in a precipitous decline in weapons production. For decades, U.S. research into the nuclear fuel cycle, and the resulting scientific expertise, had been driven by the weapons program. The sudden shift in the early '90s left a gap, and these scientific capabilities began to atrophy.

"There wasn't much hiring after me," said Crawford, who now leads ORNL's Nuclear Nonproliferation Division. "So there's a pretty hefty generational gap today in industry expertise."

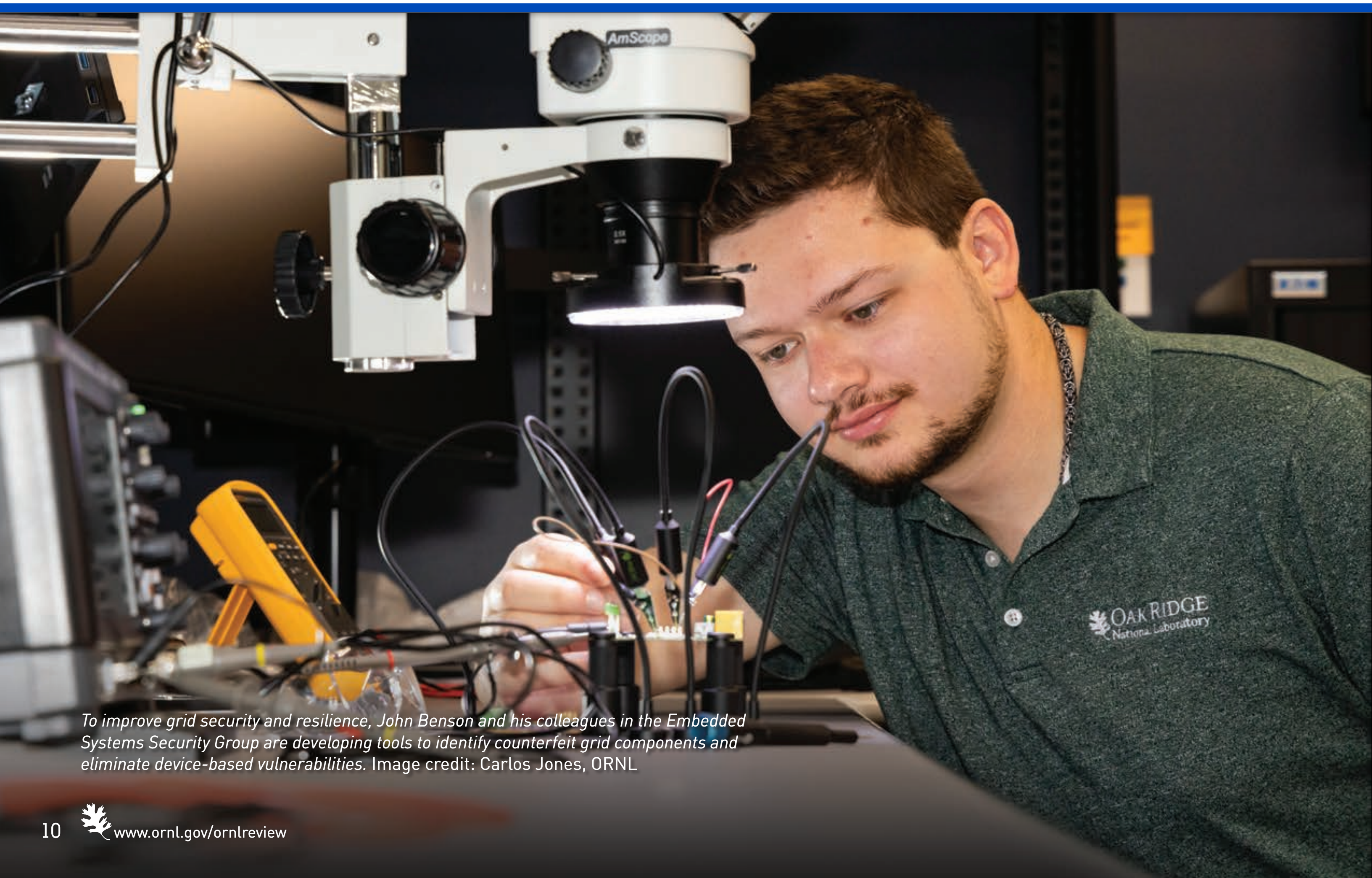
In Crawford's division, researchers, engineers and operations specialists are delivering science and technology to reduce the risk that nuclear materials will end up in the wrong hands while enabling their secure use for peaceful applications across the world.

"Whether it's early detection, real-time monitoring and accounting, or engineering for safe reactor operation, the science behind that is what we're interested in," said Jennifer Ladd-Lively, Nonproliferation Engineering Science and Technologies section head. "And we want to help move that science into practical application to better mitigate the risks."

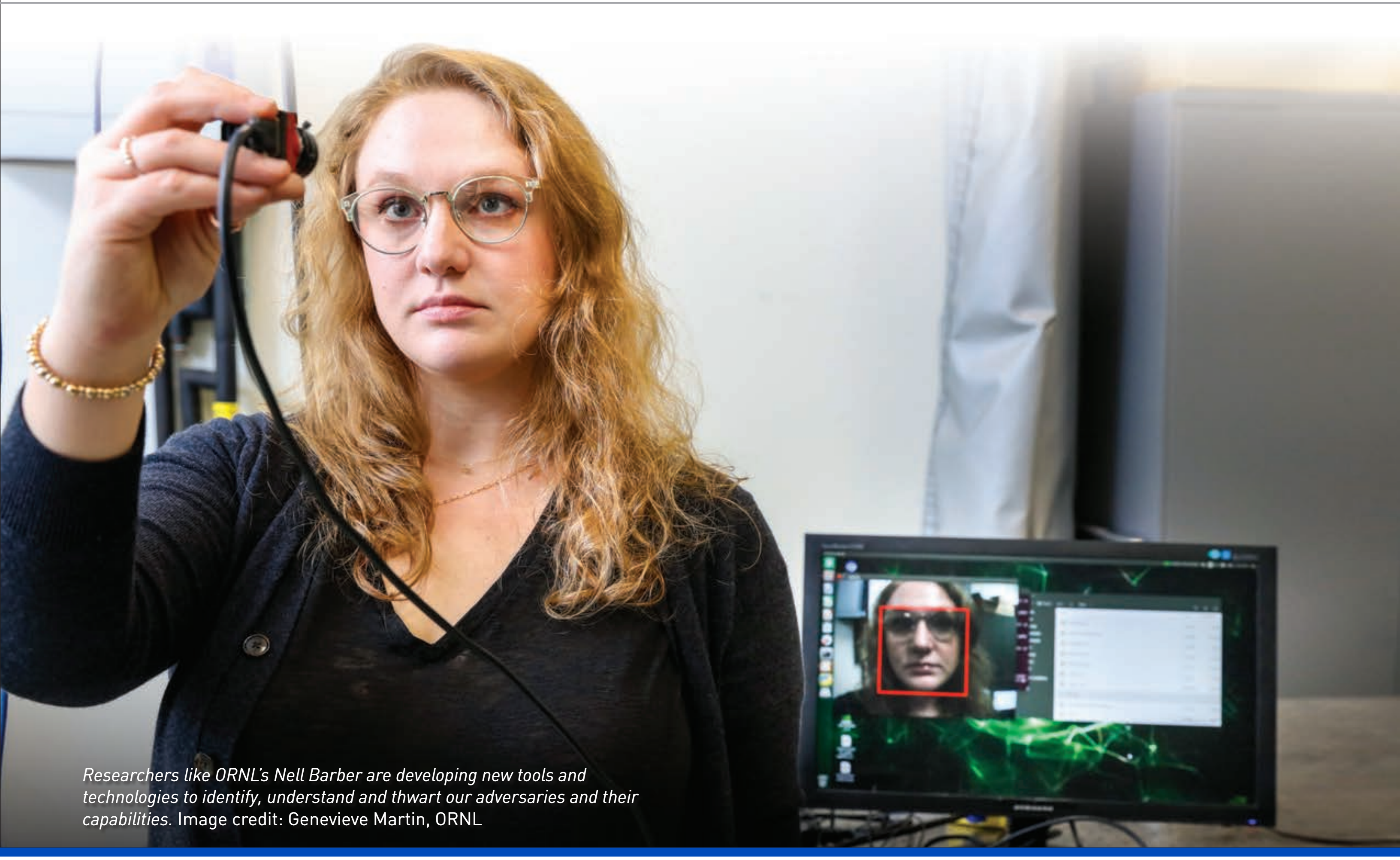
Looking to advance uranium science and fill the generational skills gap, ORNL is leading multiple efforts for the National Nuclear Security Administration's Nonproliferation Stewardship Program.

The lab is building a Uranium Science and Technology Center to reestablish core fuel cycle science and technology capabilities, advancing centrifuge modeling and simulation capabilities (see "High-performance computing boosts uranium research,"

> *"Cyber is huge, because that's the next type of warfare. With cyberattacks, you can take down entire infrastructures and destroy our ability to live the way we live. Think about your way of life; everything about your way of life involves electricity, water, infrastructure. And if you take down one of those elements, the impact is huge.*
>
> — ORNL Nuclear Nonproliferation Division Director **Cary Crawford**



To improve grid security and resilience, John Benson and his colleagues in the Embedded Systems Security Group are developing tools to identify counterfeit grid components and eliminate device-based vulnerabilities. Image credit: Carlos Jones, ORNL



Researchers like ORNL's Nell Barber are developing new tools and technologies to identify, understand and thwart our adversaries and their capabilities. Image credit: Genevieve Martin, ORNL

page 14), and developing the next generation of nonproliferation experts. Researchers are also looking at emerging technologies to ensure the U.S. is prepared to meet future nonproliferation goals and threats.

"Up until now, the nuclear industry has been slow to adapt next-generation technologies. But now we're looking at advanced manufacturing, artificial intelligence, high-performance computing," said Jared Johnson, senior nonproliferation program manager. "These tools have huge, untapped potential in our industry."

That's both exciting and concerning. For every opportunity a new technology brings to help advance the industry, reduce costs and improve security, there's an equal and opposite opportunity for those tools to be used nefariously.

The threats are evolving, and at the top of Crawford's mind are cyberattacks.

"Cyber is huge because that's the next type of warfare. With cyberattacks, you can take down entire infrastructures and destroy our ability to live the way we live," he said. "Think about your way of life. Everything about your way of life involves electricity, water, infrastructure. And if you take down one of those elements, the impact is huge."

Securing critical assets

Crawford isn't the only one thinking about cyber-enabled attacks on critical infrastructure.

Cyber Resilience and Intelligence Division Director Gleason is keenly aware of the national security threats posed by society's increasing digitization. In fact, he has a favorite analogy to explain the scope of the challenge.

Imagine you're standing beneath Niagara Falls, with a never-ending stream of water — more than 750,000 gallons per second — rushing your way. Now imagine every drop is a bit of software code, with each bit vulnerable to hacking. Where will the code lead? What will it touch? How do we find and protect the data that matters most?

"That is, in essence, the challenge cybersecurity experts face every day," Gleason said. "The amount of software generated around the world is mind-blowing, and it flows into so many different technologies and components, from smart devices and vehicles to manufacturing systems and the energy grid."

At ORNL's newly opened Cyber Science Research Facility, researchers are advancing the science of cybersecurity, leveraging artificial intelligence and high-performance computing to improve everything from cyber defense architecture to intelligence analysis.

Computer and data scientists, cybersecurity scientists, mathematicians and engineers are increasingly focused on the cyber-physical connections that make up critical national infrastructure — energy, transportation, military and manufacturing systems

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NATIONAL SECURITY SCIENCE TACKLES A NEW, page 11

— where cyber-based intrusions could produce physical catastrophes with national security implications.

As the nation pushes to modernize its energy infrastructure, the challenge of maintaining a resilient power grid grows exponentially. Each new connection to the grid, from electric vehicle charging stations to smart devices, introduces a potential vulnerability point that an adversary could exploit remotely to access the broader grid infrastructure.

To improve grid security and resilience, ORNL researchers are developing tools to identify counterfeit grid components and eliminate device-based vulnerabilities (see "Strengthening cybersecurity in the energy sector," page 20).

"We need to analyze how all these components are working together, and how that compounds functionality and vulnerability," said Tricia Schulz, group leader for Embedded Systems Security. "Our focus is on how we understand the risks and mitigate them on these devices, especially as the grid significantly expands."

> *"In my mind, the biggest threat we are facing is the increasing proliferation of emerging technologies. And it's not just proliferating to large adversarial nations; you can proliferate technologies like these everywhere and to anyone.*
>
> — National Security Sciences Associate Laboratory Director **Moe Khaleel**

Each new cyber-physical connection also generates new data. ORNL scientists are helping intelligence analysts visualize massive amounts of data that characterize how critical infrastructure is functioning and whether systems may be compromised. Leveraging ORNL's data science and high-performance computing capabilities, researchers have developed programs to fuse and analyze various forms of data in real time, helping analysts more quickly detect anomalies and threats.

They're also looking at the entities behind cyber intrusions, developing new tools and technologies to identify adversaries, understand their capabilities and thwart their attacks.

"In national security sciences, these are dynamic challenges," Gleason said. "You solve the problem one day, and the next day the adversary has adapted and moved ahead of you."

Advancing human security

Bhaduri, of the Geospatial Science and Human Security Division, wants to make sure the U.S. knows at all times what our adversaries are doing. In fact, he seeks the ability to continuously monitor the entire Earth and its systems — environmental, physical, human — much as a hospital monitors each patient's vital signs. He calls it "the pulse of the planet."

"I envision a world where anybody can wake up and say, 'I would like to know the state of my 1 km-by-1 km land I own or care about,'" he said. "What is the temperature? What is the pressure? Is it flooded? Are there people? That's the pulse of the planet."

The implications are far-reaching, and they extend beyond traditional definitions of national security. Automatic detection of wildfires and other disasters, for example, could help authorities enact efficient response plans that prioritize the populations most at risk — making communities more resilient and stable.

"One of the key objectives of national security is to minimize the loss of human lives and the damage to economies, right?" Bhaduri said. "Whether that's an active war or a battle versus diseases, resource constraints or climate disasters — they're all relevant to national security."

While the Cyber Resilience and Intelligence Division is securing individual grid connections and interactions at the component level, researchers in the Geospatial Science and Human Security Division are looking at the grid on a national scale.

With expertise in data science, high-performance computing and geospatial science, they are providing broad situational awareness of interdependent energy systems to support emergency response, disaster recovery and power restoration efforts — whether in response to adversarial attacks or extreme weather (see "ORNL tools help ensure energy supply," page 16).

While this level of situational awareness helps address immediate needs, the data it generates can also help authorities predict and prevent future events.

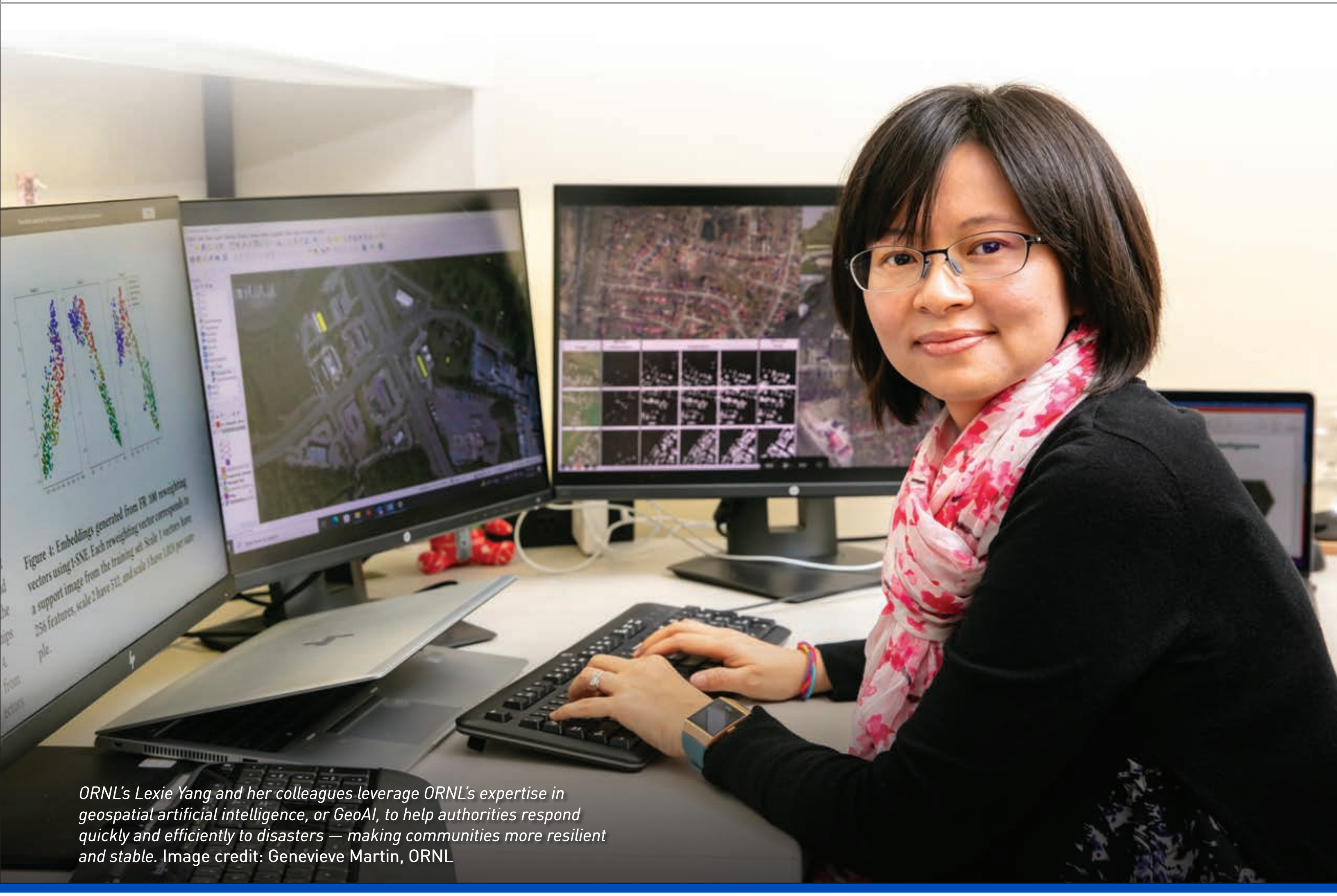
"Our ability to constantly monitor these infrastructures in a meaningful way allows us to anticipate much better," said Dave Page, who leads the Geographic Data Science Section. "We can use the data over a long period of time to understand consequences of what might happen and where we might see effects and impacts."

Yet, for all their work with global satellites, massive datasets and artificial intelligence, Bhaduri's division is ultimately focused on people. For decades, ORNL has produced LandScan, the definitive global population dataset for human dynamics and distribution modeling. LandScan has been used around the world to estimate populations at risk and aid in disaster planning and response.

"If you have a good sense of where people were at the time of an event, you have a very educated guess as to how many people may have been affected in a particular location," said Marie Urban, Human Geography group leader at ORNL. "From there, you can adjust the level of response and assistance for the greatest impact."

The unique integration of these capabilities and datasets — along with resources like a new, small satellite ground station and access to the world's fastest supercomputer, ORNL's Frontier — can significantly reduce the amount of time it takes to get from data to decisions to action.

For disaster scenarios, Bhaduri and team aim to produce meaningful information within the first 72 hours, the crucial period



ORNL's Lexie Yang and her colleagues leverage ORNL's expertise in geospatial artificial intelligence, or GeoAI, to help authorities respond quickly and efficiently to disasters — making communities more resilient and stable. Image credit: Genevieve Martin, ORNL

during which responses can save lives. That — saving lives — is their key metric.

"In the end, if we cannot really move that needle, all we have are some great sets of PowerPoint slides and a few papers," Bhaduri said.

Confronting emerging technologies

As Gleason noted, the challenge in national security science is that there's always someone on the other side trying to push that needle back. The adversary's task gets easier as disruptive technologies — artificial intelligence, autonomous systems, biotechnology — become more widely available.

"In my mind, the biggest threat we are facing is the increasing proliferation of emerging technologies," National Security Sciences Associate Laboratory Director Khaleel said. "And it's not just proliferating to large adversarial nations; you can proliferate technologies like these everywhere and to anyone."

To address the challenges of distributed, emerging technologies, Khaleel believes we should treat them similar to nuclear materials and take a cue from the international nonproliferation regimes established to monitor, regulate and control them.

"Cyber, for example, is a weapon, so how do you ensure that others don't have these capabilities?" Khaleel said. "The other thing is to think about economic security. You don't want these technologies that give the United States economic advantage to just walk out of the country."

What's more, Khaleel said, the U.S. must continually evolve its own capabilities to ensure we outpace our adversaries. He points to an emerging field ORNL researchers are exploring, cognitive AI, as an example.

"The nature of cyberattacks will continue to evolve. When these things evolve, we cannot just have static AI-based defense schemes. We need resilient, cognitive AI that continues to evolve with the threats."

With its combination of historical expertise, world-class research facilities and translational science capabilities across diverse disciplines, ORNL is uniquely suited to solve the modern challenges of national security. But what really sets ORNL apart, Khaleel believes, is its people.

"From our analysts to our teams working in nonproliferation, cyber and human security, along with researchers across the lab engaged in national security missions, we have great people. I think that's our secret in this lab; we have great people who are passionate about what they do and believe in one another."

High-performance computing boosts uranium research

by Liz Neunsinger
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Consider the way air flows over an airplane wing, how slight variations in design allow the plane to take off or keep it on the ground.

The first airplane wings looked very different from what they do today, as engineers have come to understand the fluid dynamics of air flow and computer simulations have helped reveal how even a slight design change can optimize the performance of a dynamic system.

In the same way, use of supercomputers at ORNL to simulate fluid dynamics in gas centrifuges is revitalizing uranium science research in the United States.

Gas centrifuges are used to create low-enriched uranium for nuclear power but can also create highly enriched uranium for nuclear weapons. (Enrichment refers to how much of a quantity of uranium is the isotope uranium-235.)

The creation of physics-based gas centrifuge simulations to better understand centrifuge design for uranium enrichment is the primary purpose of a program called the Advance Simulation Initiatives for Nonproliferation Applications, or ASINA. These simulations will enable scientists and engineers to better inform policymakers regarding nonproliferation missions.

After Oak Ridge built the world's first plutonium production reactor — the Graphite Reactor — during World War II's Manhattan Project, the U.S. nuclear weapons program grew in capability and expertise for four decades. But, as priorities shifted following the end of the Cold War, that scientific advantage diminished. The scientists and engineers behind ASINA intend to get it back.

"Today, there are key gaps in our technical understanding of the performance and proliferation capabilities of certain centrifuge designs," said Jared Johnson, Uranium Science and Technology program manager at ORNL. "ASINA and related efforts will close that gap and give the nation the ability to reliably analyze, assess and predict centrifuge performance and operations."

Behind ASINA is a multidisciplinary team of engineers and scientists who understand computational science, fluid dynamics, multiphysics coupling, materials science and isotope enrichment. It takes these different areas of expertise to create a computer simulation capable of handling the various computational scenarios needed for gas centrifuge research — a mix of expertise readily available at ORNL.

"ORNL has historic strength in uranium enrichment, having the centrifuge program here for decades," said Matt Bement, deputy principal investigator for ASINA. "With the HPC and code-development experience, Oak Ridge is the most logical place to do this."

Using computers to simulate gas centrifuges is not new; code for modeling these centrifuges has been around since the 1970s. Today's software engineers are dusting off the old code and boosting it with a much-needed upgrade to leverage the speed of high-performance computing and the intelligence of machine-learning algorithms.

"ASINA gives us an opportunity to explore things that we can't do or can't see experimentally," said Franklin Curtis, ORNL Flow, Thermal, and Data Science Group leader, referring to the expensive and time-consuming process of building physical centrifuge plants and running individual experiments. "Having a better

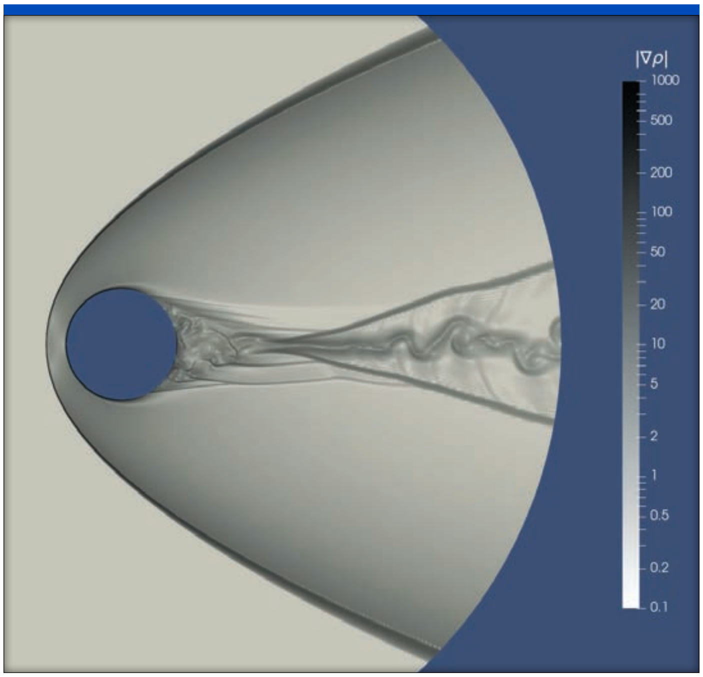

Image from an ASINA simulation illustrating flow past a cylinder.
Image credit: ORNL

simulation capability gives us this new insight into how these very simple-sounding but complicated processes work."

Results can be delivered within a few seconds or hours to collaborators anywhere in the U.S., and these new insights could help researchers and analysts better understand an adversarial nation's ability to enrich uranium beyond the 3 to 5 percent needed for nuclear energy.

2D and 3D models are among ASINA's key outputs. Using computational fluid dynamics, the models answer questions about internal flow in a gas centrifuge. Simulations show different gas speeds, turbulence and pressure changes, as well as the resulting effects on internal gas dynamics. Researchers can run thousands of simulations at once, each with a tiny difference, to see how outcomes change.

2D modeling has long been part of the gas centrifuge research program and remains a significant part of today's research, albeit with greater compute power. Small 2D calculations can be run on a desktop computer; however, more challenging tasks, such as quantifying uncertainty in predictions with multiple inputs, need significantly more power. Having the ability to run thousands of calculations on supercomputers can mean producing results promptly enough to effectively influence decision-making.

3D modeling is another challenge altogether, but the benefits of 3D simulation will be a gamechanger for those working to understand how objects actually move along multiple planes. Greg Davidson, senior researcher for the HPC Methods for Nuclear Applications Group, believes 3D will put high-fidelity modeling at the fingertips of centrifuge engineers. The challenge of 3D is that researchers need very powerful computers to run the calculations efficiently.

"When you add that extra dimension, the computer you need gets a lot bigger, and how you write your code has to be very thoughtful," said aerospace research scientist Ryan Glasby. 3D calculations will be at least 1,000 times harder than 2D calculations, he said, and will require leveraging HPC to meet the demands of additional computational power.

In addition to ASINA's implications for global nuclear nonproliferation, the program will improve domestic uranium capabilities, such as carbon-free nuclear power and medical isotopes. Engineers are diving into the future of gas centrifuge design mechanics and building the ability to identify weaknesses in materials or system design.

Gas centrifuges are costly. Simulating gas centrifuge behavior allows engineers to test designs before construction by conducting trials in a mock environment, accounting for risk and tolerance in the manufacturing process.

The ASINA program is one of two efforts ORNL is leading for the National Nuclear Security Administration's Nonproliferation Stewardship Program. The other, the Uranium Science and Technology Center, is building unique laboratories and test beds that will allow the research community to advance the state of the art in uranium sciences. Together, ASINA and USTC will also focus on building the next generation of U.S. nonproliferation experts.

The DIRAC Collateral System (pictured) and NARSIL Moderate System support ASINA modeling and simulation efforts
Image credit: Carlos Jones, ORNL

Flow, Thermal, and Data Science Group Leader Curtis and his colleagues are proud to build on the country's uranium science legacy to revive and advance the field. They are working to take centrifuge technology, a consistent part of the nuclear science industry since the 1950s, and use it to advance uranium's place in the peaceful use nuclear energy for economic and medical progress.

"We're setting the stage to allow the United States to become independent of isotopes from other countries and to be able to continue on the legacy that the people here at the lab in the past have done," Curtis said.

ORNL tools

help ensure energy supply

by S. Heather Duncan
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In May 2021, a cyberattack on the Colonial Pipeline Co. triggered soaring gas prices and shortages at East Coast gas pumps. Thanks to geospatial researchers at ORNL, the government understood how the pipeline shutdown affected crude flows and refinery operations.

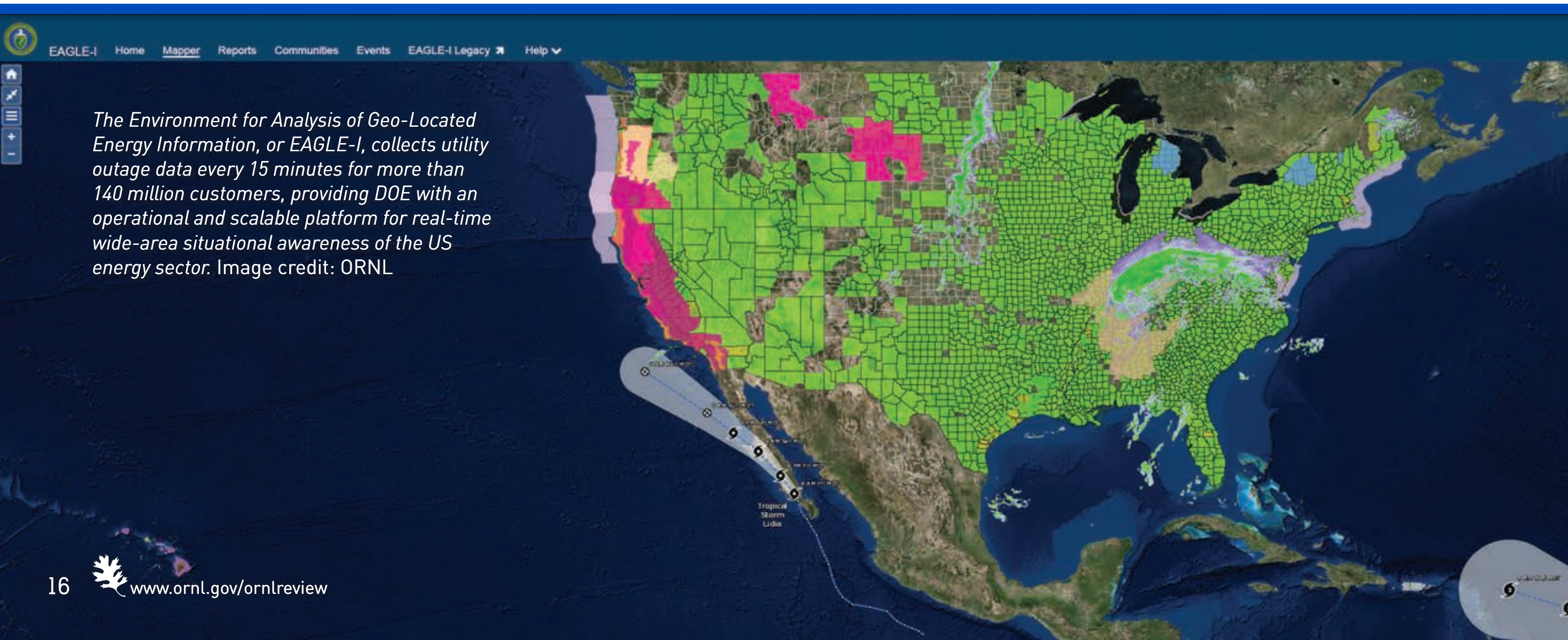
But it couldn't tell how shortages would play out at gas stations in specific regions. During some types of national disasters, that information could save lives.

"During a hurricane event, if we expect people to evacuate, they need access to gasoline and diesel," said Bandana Kar, who leads ORNL's Built Environment Characterization Group. "We are developing models in collaboration with the National Energy Technology Laboratory to understand which gas stations are going to run out of fuel faster based on their capacity, location, supply and demand in the area."

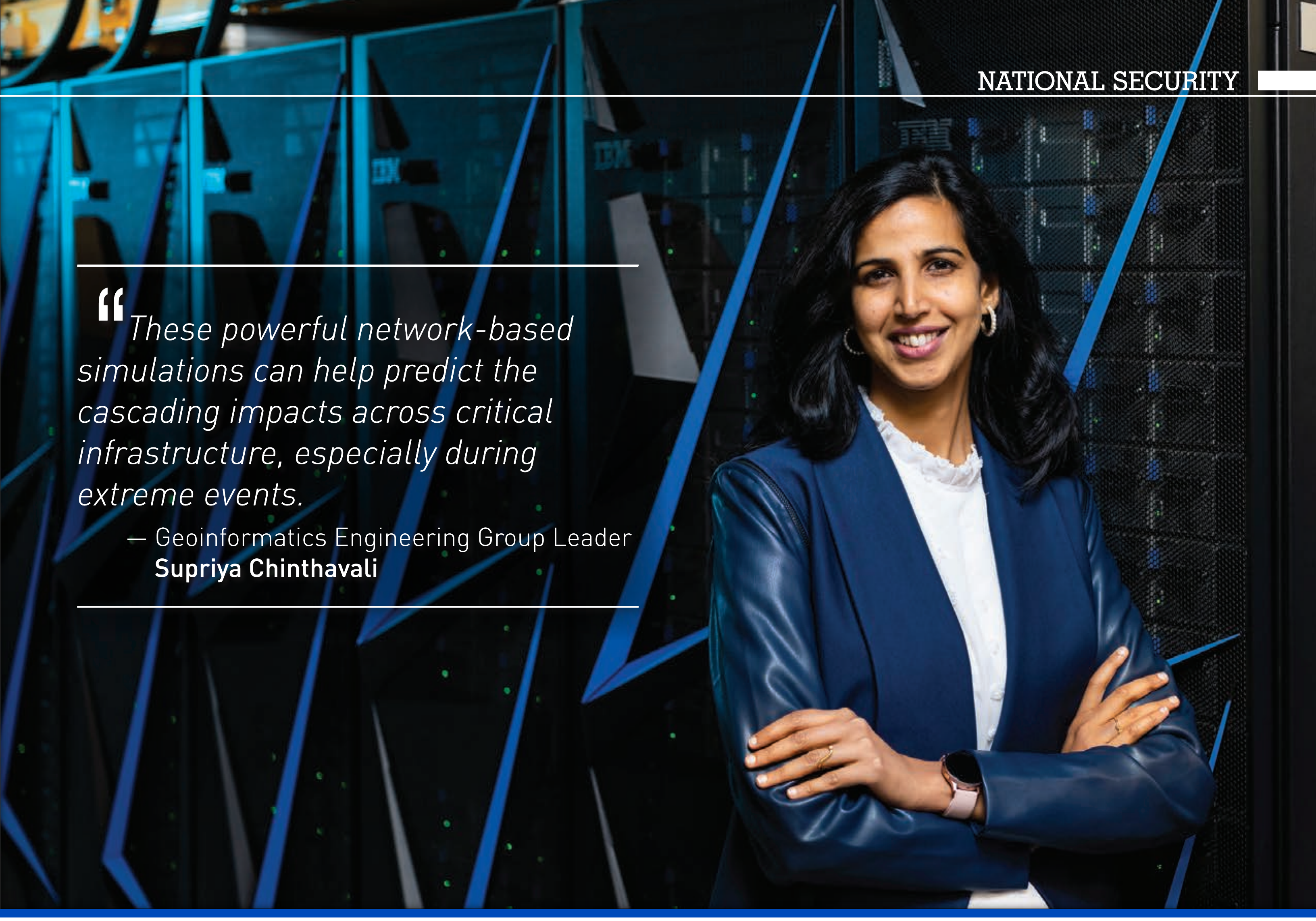
Disruptions to interconnected energy systems, whether caused by weather or attacks, are a major threat to national security. Resilient, robust energy infrastructure protects human life as well as the functions that underpin society, including health care, transportation and communications.

ORNL's Geospatial Science and Human Security Division combines expertise in high-performance computing and geospatial science to provide decision-makers with timely information for rapid emergency response, disaster recovery and power restoration. ORNL data, tools and analysis support resource planning in case of large-scale outages caused by extreme events due to climate change.

"We are basically taking a broad view to understand on a daily basis: What is happening on the ground with regard to energy supply?" Kar said.



The Environment for Analysis of Geo-Located Energy Information, or EAGLE-I, collects utility outage data every 15 minutes for more than 140 million customers, providing DOE with an operational and scalable platform for real-time wide-area situational awareness of the US energy sector. Image credit: ORNL

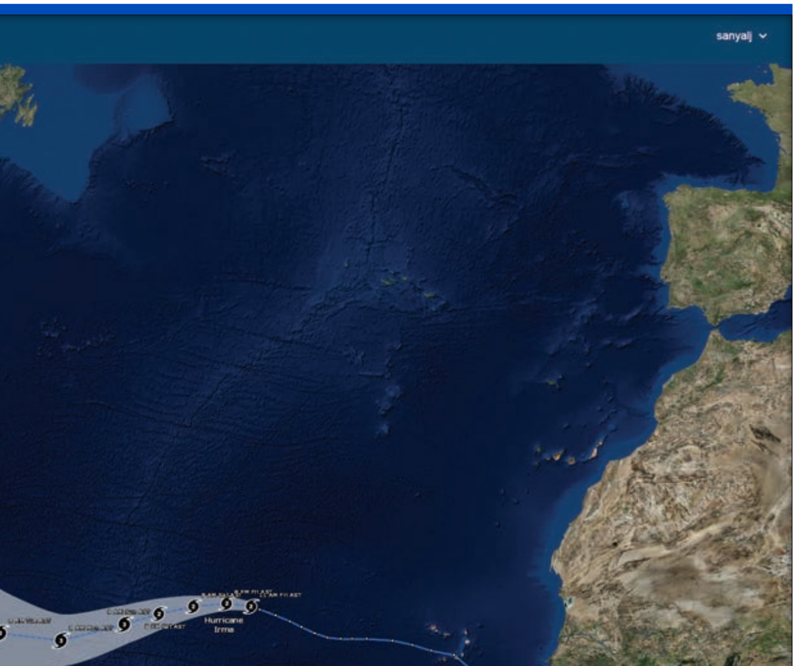


"These powerful network-based simulations can help predict the cascading impacts across critical infrastructure, especially during extreme events.

— Geoinformatics Engineering Group Leader **Supriya Chinthavali**

Understanding energy interdependencies

To support responses to future scenarios like the Colonial Pipeline attack, Kar and her colleagues have developed a supply chain model — the Situational-Temporal Awareness Tool for Integrated Oil and Natural Gas Systems, or STATIONS — that determines petroleum supplies all the way from refineries to fuel loading facilities to the pump, to help with petroleum demand during extreme events. Emergency responders and utilities can use the model to address resource planning.



STATIONS results will be incorporated into a larger real-time situational awareness tool hosted by ORNL: the Environment for Analysis of Geo-located Energy Information, or EAGLE-I, a program in DOE's Office of Cybersecurity, Energy Security, and Emergency Response. It is the authoritative federal source for monitoring energy infrastructure, reporting live outages, displaying potential threats, modeling to prepare for future scenarios and coordinating emergency response and recovery.

But oil and natural gas are just two U.S. energy resources, and they come from different sources and move through separate management and distribution networks. ORNL experts can integrate system status and supply chain information from oil, gas and electric systems to understand how those networks are intertwined.

For example, a hospital that loses electricity during an ice storm must then rely on diesel fuel to power its generators. This will lead to a spike in petroleum demand in the area. If the petroleum supply chain is unprepared, the hospital might struggle to find a gas station with the diesel needed to keep life-saving machines operating until electricity is restored.

See ORNL TOOLS HELP ENSURE ENERGY SUPPLY, page 18

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URBAN-NET is a tool developed by ORNL scientists that represents these interdependencies in energy distribution as a networked graph, visually displaying vulnerabilities as analysts run different scenarios. URBAN-NET is also a component of EAGLE-I.

"These powerful network-based simulations can help predict the cascading impacts across critical infrastructure, especially during extreme events," said Supriya Chinthavali, group leader for Geoinformatics Engineering. If a natural gas transmission line fails, for instance, which natural gas power plants will be at risk? What are the worst-case downstream results, such as widespread power outages or hospitals at risk?

New datasets and geospatial overlays can be added to understand the growing risk posed by developing hazards. For example, a severe drought could be layered onto the map, along with data about wildfire locations and National Weather Service warnings, to identify energy infrastructure facing the most stress, demand and risk.

Monitoring outages and restoring power

EAGLE-I delivers updates every 15 minutes on where outages are occurring and how many people are without power across the country. It plays a critical role for DOE in the National Response Framework, said Aaron Myers, ORNL EAGLE-I technical lead.

"EAGLE-I provides a national-scale situational awareness platform for sharing data across the energy sector," Myers said. "Outputs from EAGLE-I have been used across various response efforts, and it has become a key application in the (national) response effort."

Real-world impacts

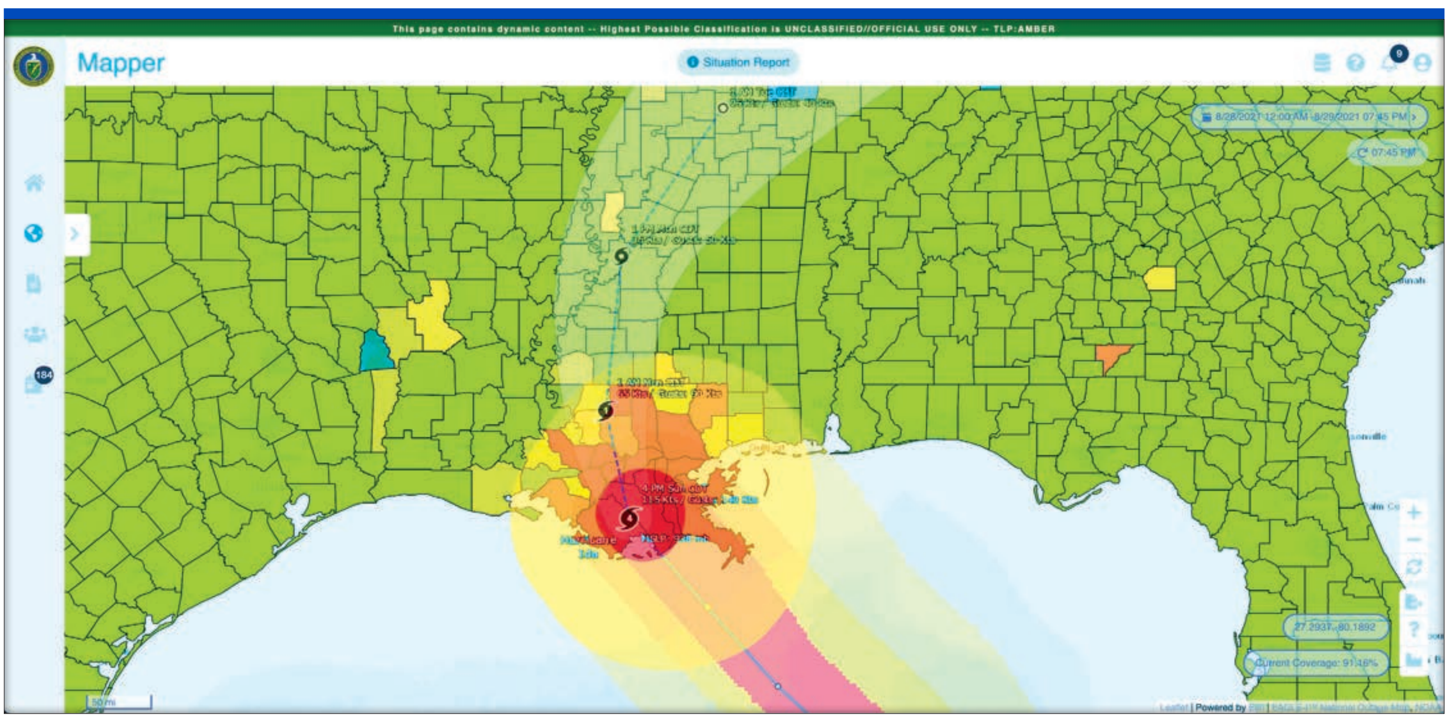
ORNL's critical infrastructure resilience tools and models have supported emergency response and energy restoration after many recent disasters:

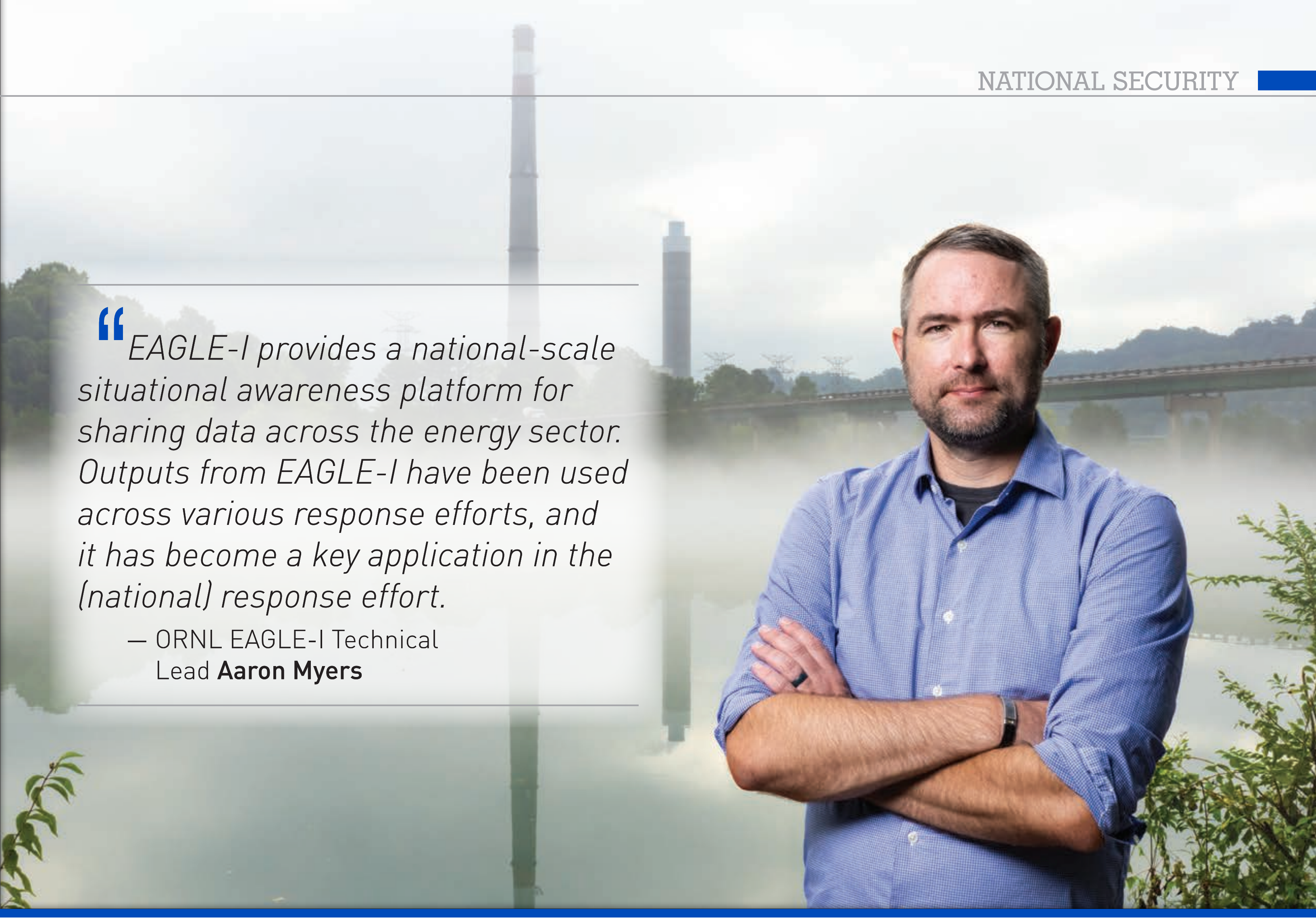
- Colonial Pipeline ransomware attack
- California wildfires
- Extended electricity outages during 2021 Texas cold snap
- Redesign of Puerto Rican electricity infrastructure after Hurricane Maria
- Northeastern blizzards and ice storms
- Winter 2021 tornados and summer 2022 flooding in Kentucky

But EAGLE-I doesn't indicate how long the outages might last. Not all electricity companies report when they expect power to be restored, and no standardized format exists for those that do, Chinthavali said.

To address that problem, ORNL spearheaded the Outage Data Initiative Nationwide, or ODIN. Starting with a pilot program in Washington state, emergency management agencies, a handful of utilities and vendors worked toward standardized outage data reporting. Now more than 60 utilities report standardized outage information to ORNL, which collates the data into a map that enables power companies to quickly see both their own outages and

A screenshot of the EAGLE-I platform when Hurricane Ida made landfall near New Orleans as a Category 4 storm in August 2021. The colors represent the percentage of electric utility customers without power by county. The platform updates every 15 minutes and served as the official source for outage data in support of the federal response effort, helping emergency responders identify areas of impact and understand the magnitude of outages across the region. Image credit: ORNL





> *"EAGLE-I provides a national-scale situational awareness platform for sharing data across the energy sector. Outputs from EAGLE-I have been used across various response efforts, and it has become a key application in the (national) response effort.*
>
> — ORNL EAGLE-I Technical Lead **Aaron Myers**

those at neighboring utilities to help predict where backup crews might be available.

"ODIN enables utilities to be more efficient in restoring power through better management of mutual aid," Chinthavali said.

Almost 10 years of EAGLE-I power outage data provides historical records that can be used to predict future outages and their lengths. This type of analysis could help federal agencies better support communities with a history of long outages, for example by preventing deaths when home medical devices stay shut down too long.

While this risk has been reduced as backup options have become more accessible, these resources still last for a limited time.

"Historically, after that, people start dying," Chinthavali said. "It has happened so many times, especially during hurricanes. So it's very important to estimate restoration times at the local level, to make sure the right help arrives in time to save people's lives." ORNL experts have begun working with the Federal Emergency Management Agency to develop a system for creating those estimates.

Advancing climate security and energy justice

U.S. agencies are increasingly recognizing and preparing for the ways climate change may affect national security, including risks to power distribution. Chinthavali's team works with ORNL climate scientists to study the effect on energy infrastructure if climate change multiplies the effects of extreme weather events as expected, and it plan strategies for coping with these events. For instance, how would the grid deal with twice as many hurricanes? As we face more heat waves and wildfires, which areas are most likely to face rolling blackouts?

Kar said energy justice is likely to be an expanding challenge as climate change intensifies. For example, energy suppliers need to understand how climate-induced migration will shift energy demand, and which populations will face rolling blackouts because of extreme weather. EAGLE-I demographic and historical data could be used to identify communities that lack access to reliable power.

"We can see which areas are experiencing energy burden through longer and more frequent outages," Kar said, "either because they are rural, or they have aging infrastructure, or they don't have an alternate source of energy."

When alternate energy sources are added to address these weaknesses, they need to be strategically placed on the grid. ORNL experts help electric utilities with this process through analysis of real-time power flow and load loss.

The challenges of distributed energy, the grid edge, energy justice, and climate change are expected to grow. ORNL scientists are preparing for them, as well as for unexpected disasters and attacks, to protect American security by keeping energy flowing.

Strengthening cybersecurity

in the energy sector

by S. Heather Duncan
duncansh@ornl.gov

Almost every online shopping site influences buying decisions by providing a rating system for its products. Five stars? Looks like a good buy. One star? Maybe it's good enough for what I need.

Similarly, government-backed certification programs like ENERGY STAR offer clarity by vetting specialized claims against a formal set of standards.

Researchers at ORNL are working on a certification system for one of the biggest emerging needs facing electric utilities: cybersecurity.

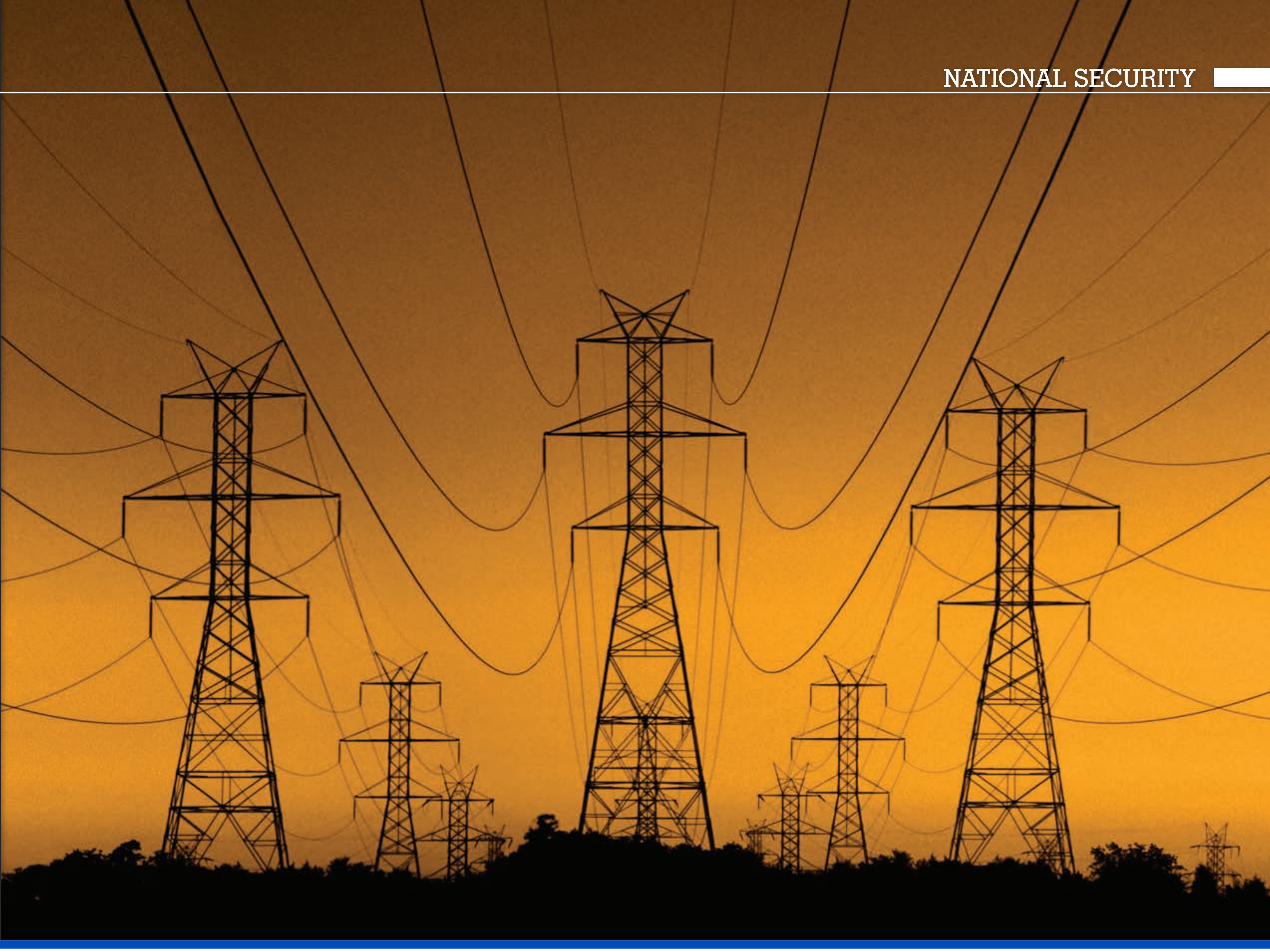
Energy infrastructure is so interconnected that cascading failures can have wide-reaching effects on access to safe food, winter heating and life-sustaining medical devices. Recognizing this, companies selling components for the grid tout an array of features to strengthen it against cyberattack. But utilities can have difficulty navigating this barrage of marketing about new product features.

> *"Think of all the vulnerabilities that have been found in the past five or 10 years. If systems aren't updated, many of those might still be around in our critical infrastructure. Can we update the equipment to eliminate those vulnerabilities without causing unacceptable downtime?*
> — ORNL Embedded Systems Security Group Leader **Tricia Schulz**

The cybersecurity certification system under development at ORNL will quantify the value and effectiveness of security features, letting utilities understand the strength and weakness appropriate to meet their cybersecurity needs.

ORNL's Cyber Resilience and Intelligence Division also helps energy companies find bugs, knockoff parts, undocumented functionality and other cyber weaknesses in equipment already operating.

Juan Lopez leads the Energy and Control Systems Security Group.
Image credit: Carlos Jones, ORNL



Unlike personal electronics, most energy infrastructure components have a long life cycle. That means cyber weaknesses can last decades or arise while old technology is still being used, explained Tricia Schulz, group leader for Embedded Systems Security.

"Think of all the vulnerabilities that have been found in the past five or 10 years. If systems aren't updated, many of those might still be around in our critical infrastructure," Schulz said. "Can we update the equipment to eliminate those vulnerabilities without causing unacceptable downtime? How do we plan to do that for the weaknesses we find in the next 10 years?"

Validating cybersecurity claims

To address these challenges in the short term, some suppliers offer cybersecurity upgrades.

"They advertise features but don't tell you the level of robustness," explained Juan Lopez, group leader for Energy and Control Systems Security.

For example, a utility could pay extra for a password system controlling login access to remote equipment without understanding how much protection they'll receive. Password options can range from a basic three letters to a much more secure combination of numbers, digits, and symbols with a lockout feature for failed attempts.

"We're trying to come up with a star rating for truth in marketing," Lopez said. "It's a win-win for the manufacturers that make the components and the customers that buy them."

Vendors benefit from quality differentiation. Users benefit from consistent and assured performance.

ORNL scientists are piloting a star rating for three types of products or security features: passwords, real-time automation controllers and secure shell; these act as an encrypted tunnel for network services. Such features are commonly available or can be easily added with an upgrade to firmware, the code embedded in network-connected devices. The rating scale would award one star to products with minimal cybersecurity and four or five stars to the most robust.

"And companies can decide whether that level of protection is needed, so you can tailor your spending to your actual needs," Lopez added.

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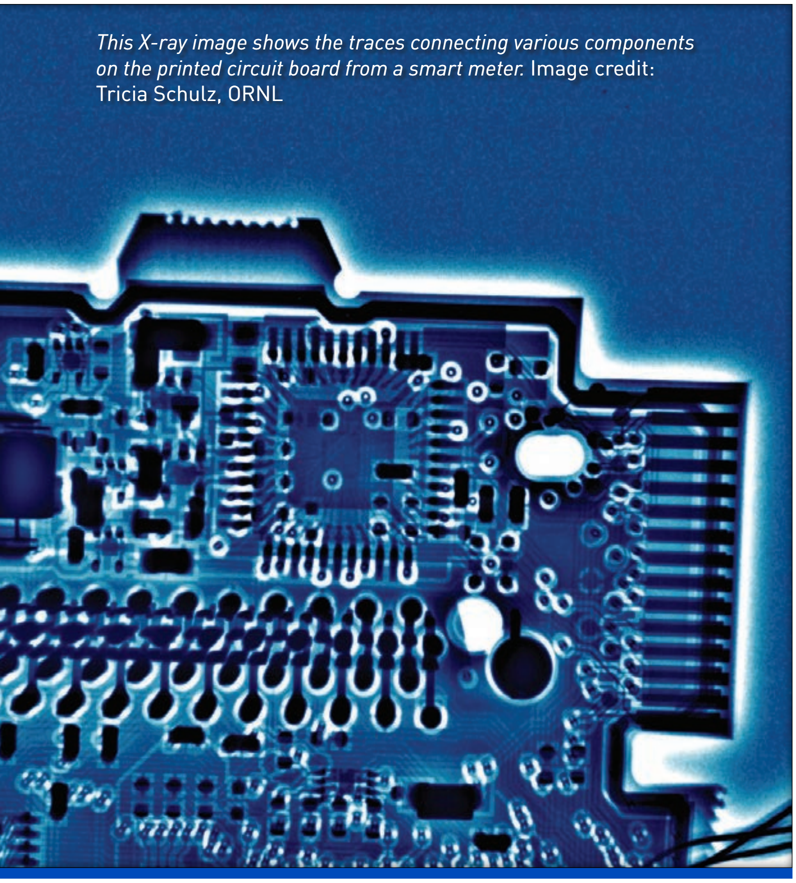


This X-ray image shows the traces connecting various components on the printed circuit board from a smart meter. Image credit: Tricia Schulz, ORNL

STRENGTHENING CYBERSECURITY IN THE ENERGY SECTOR, page 21

The framework, based on proven compliance certification approaches like ENERGY STAR, uses a semiautomated process to verify product performance in a hardware test bed. The system can be scaled up to large grids or down to microgrids.

The testing framework could eventually be used by a third party to run the rating program, said Lopez, who provided a demonstration to several public utility partners in September. The project was funded by DOE's Cybersecurity for Energy Delivery Systems R&D program.

Finding fakes through "fingerprints"

Cyber challenges to the supply chain continue after purchasing, though, and ORNL researchers are also ferreting out vulnerabilities after components have already been bought or installed. In some cases, nefarious tampering may have added bugs or secret functions. In others, a replacement part might just be cheap junk that looks like the real thing.

"In the power grid, I'm worried about both problems," Lopez said. "Counterfeit components are being purchased legally and installed in critical infrastructure as companies do repair and replacement. These knockoffs may be less safe." For example, a counterfeit version could explode because it can't take the same heat and pressure as the more robust original.

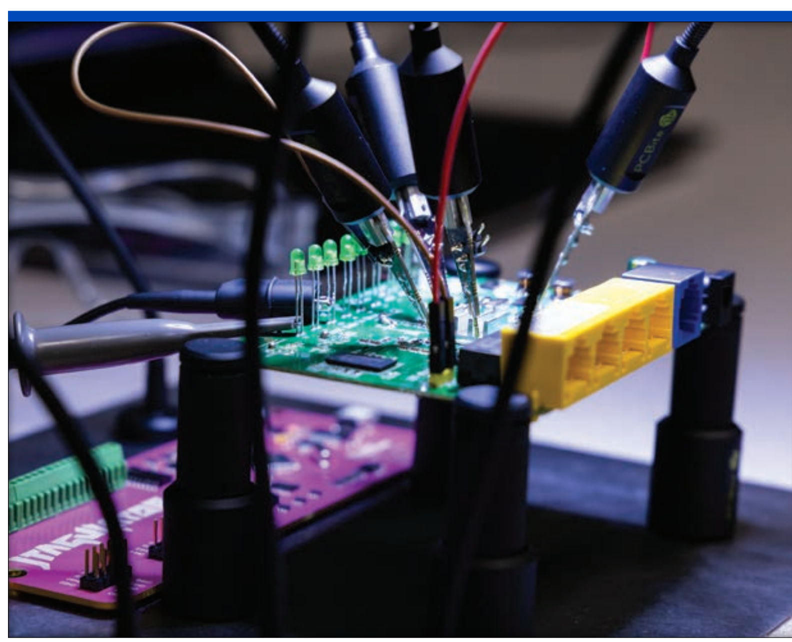
"The operator who has this in his system has no way to differentiate the products," Lopez said.

To solve this problem, Lopez's group has developed a handheld tool to verify parts in inventory or even while operating. The tool aims ultra-wideband signals at a component, which don't interfere with its internal systems. When these signals bounce back, returning waves are detected using small-aperture radar. A mathematical process removes background noise from the signal. The result is a type of 3D signature for each component.

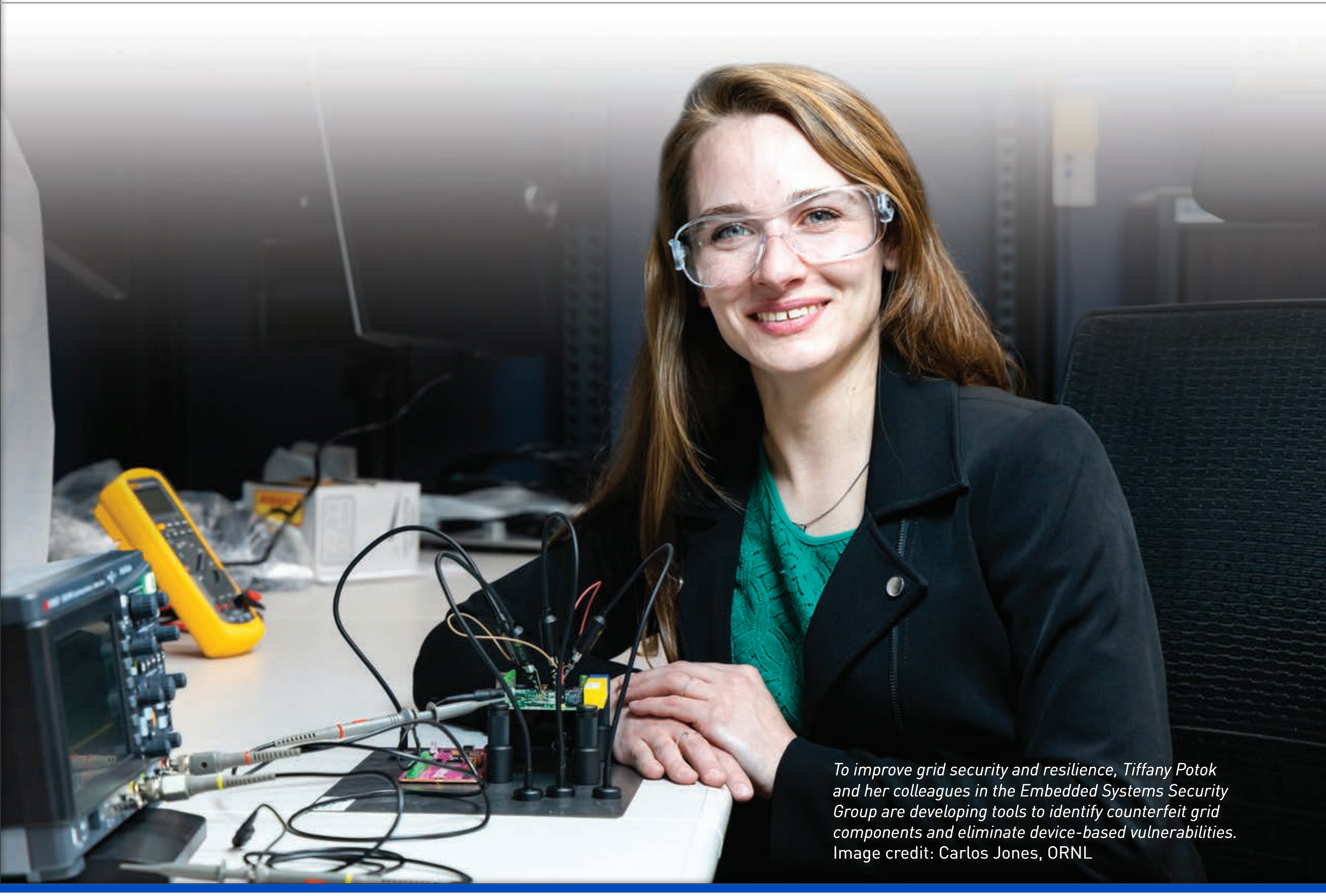
> *"Counterfeit components are being purchased legally and installed in critical infrastructure as companies do repair and replacement. These knockoffs may be less safe.*
>
> — ORNL Energy and Control Systems Security Group Leader **Juan Lopez**

"The idea came from a technology that has been around for years: This needs to be like fingerprints," Lopez said. "Once you get even a partial fingerprint, you can still get a match. If you don't have a match, what you have is probably counterfeit, and you need to investigate further."

The tool can also be used to check whether a part has changed since installation. "A utility can scan hundreds of devices and determine fairly quickly if they match," said Lopez, adding that the Tennessee Valley Authority has expressed interest in field-testing this technology as well.



Oscilloscope probes in the Embedded Systems Laboratory are attached to a printed circuit board for signal analysis. Image credit: Carlos Jones, ORNL



To improve grid security and resilience, Tiffany Potok and her colleagues in the Embedded Systems Security Group are developing tools to identify counterfeit grid components and eliminate device-based vulnerabilities. Image credit: Carlos Jones, ORNL

Understanding firmware, hidden functions and the Smart Grid

ORNL scientists are also working to identify, understand and eliminate other device-based vulnerabilities that could harm energy infrastructure. They analyze hardware, software and firmware, investigating the capabilities of all the components within a device.

"It's often cheaper for companies to reuse a printed circuit board design and only use components of the software they need than to make a new version of the board," Schulz said. "That doesn't mean the other functionality doesn't exist." Hostile actors could activate those latent functions to cause the device to fail, behave in an unexpected way or open a door to cyber intrusion.

Schulz's group also partners with the Vulnerability Science Group at ORNL to study the security of firmware embedded inside internet-networked consumer devices such as appliances and thermostats, often called the Internet of Things, or IoT. These edge devices, too, may have capabilities that aren't initially active or obvious, such as microphones in home security systems.

"Sometimes vendors include hardware that can expand a device's capability with a future software release, but if that functionality is not obvious at the time of purchase, then it is difficult to fully understand the risk," Schulz says. "Similarly, we need to understand the software and its potential weaknesses."

To improve understanding of device firmware, the Vulnerability Science Group developed a process that enables experts to find and mitigate vulnerabilities before firmware is deployed into critical systems such as the power grid.

While these types of vulnerabilities might concern individual homeowners, the networking of such devices can broaden their potential for damage. Their cyber weaknesses could be leveraged to interfere with how the electric grid operates internally or to create unexpected power fluctuations.

For example, a vulnerability in widely used electric vehicle charging equipment could be used to trigger a sudden, huge power draw.

"It's almost an overwhelming problem," Schulz said. "Chargers are in people's houses. How do you find all the owners? How do you tell all the owners they need to update?"

Her team works on mitigating such vulnerabilities. "We are moving toward a smart grid," she said. "You have this whole chain of different devices that are increasingly able to communicate over the internet. Being able to understand the risks associated with that, and to reduce those risks, is important."

Engineers and scientists

support nonproliferation efforts

by: Liz Neunsinger
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Jason Oberhaus figures nobody studies engineering to become an intelligence analyst.

Yet he and his team of scientists and engineers in ORNL's Fuel Cycle Analysis Group have been using their technical insights to support the lab's national intelligence missions for years.

They're part of a little-known legacy of engineers becoming intelligence-producing professionals that dates back to World War II.

The Manhattan Project drew scientists and engineers in many disciplines from across the country to swiftly advance understanding of atomic energy and develop the world's first nuclear weapons. A lesser-known mission during the last two years of the war saw some of those same American engineers traveling around Europe to understand the state of the Nazi nuclear program.

This latter effort, known as the Alsos Mission, "recognized that people in R&D were essential to helping the intelligence people understand what the enemy was doing," said Chuck Durant, director of ORNL's Field Intelligence Operations Division.

These R&D experts were trained in the scientific method, not warfare or spycraft. But they joined a team of soldiers drifting through towns in Europe collecting information on the people and capabilities of Germany's nuclear program. It was an important lesson that continues to shape the DOE's approach to nuclear intelligence today.

"It's a lot easier to teach a scientist how to do intelligence work than it is to teach an intelligence analyst Ph.D.-level science overnight," Durant said.

Today, a team of engineers at ORNL carries on the legacy of the Alsos mission, ensuring nuclear fuel cycle expertise is a part of the national security decision-making process.

"We bring subject matter expertise to help the Intelligence Community solve nuclear nonproliferation challenges," Oberhaus said. "We're providing unique technical analysis and articulating these things to policymakers in a way that helps them understand the risks and the implications."

British and American members of the Alsos Mission in April 1945 dismantling the German experimental nuclear reactor in Haigerloch. Image credit: U.S. Army

Members of the Alsos mission uncover uranium cubes hidden by German scientists in a field in Haigerloch, Germany, toward the end of World War II. Image credit: U.S. Army

ORNL's fuel cycle analysts have played an important advisory role in several nuclear-related negotiations between the U.S. and foreign nations. Here, John Kreykes, right, discusses Libyan nuclear technology with then-President George W. Bush during a visit to Oak Ridge in 2004. Image credit: Lynn Freeny, DOE

Professionals who have participated in research, worked in nuclear facilities and handled nuclear equipment and materials have the experience needed to keep vital nuclear and radiological materials out of the hands of people who want to make bombs and other dangerous devices.

Even with years of real-world experience, the road from engineer to analyst isn't easy. The Intelligence Community has its own unique set of standards and methods engineeers must learn.

"We teach them intelligence tradecraft — how to do the intelligence, how to write the reports," Durant said. "We continue the tradition of deploying ORNL's expertise in science and research to support policymakers at the highest levels."

Leveraging open science research to solve challenges facing the nation today, ORNL can offer scientific expertise in areas outside the nuclear fuel cycle. Capabilities in innovative materials, high-performance computing, neutron research, sensors, robotics, cybersecurity and artificial intelligence aid in promoting resilience in economic and military industries.

Samuel Goudsmit and Frederic Wardenburg, at left, of the American Alsos Mission sit across from Eric Welsh and Rupert Cecil of British Intelligence at the headquarters of the German Army's fission program. Image provided courtesy of Brookhaven National Laboratory

"Science and technology are becoming more and more integral to national security," said Durant. "We're contributing in real time to help national policymakers understand some of the most complex challenges in our world."

Summit study tackles superconductivity

by Matt Lakin
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A study led by ORNL researchers used the lab's Summit supercomputer to close in on superconductivity, a central challenge of modern physics whose solution could usher in the next generation of energy technologies.

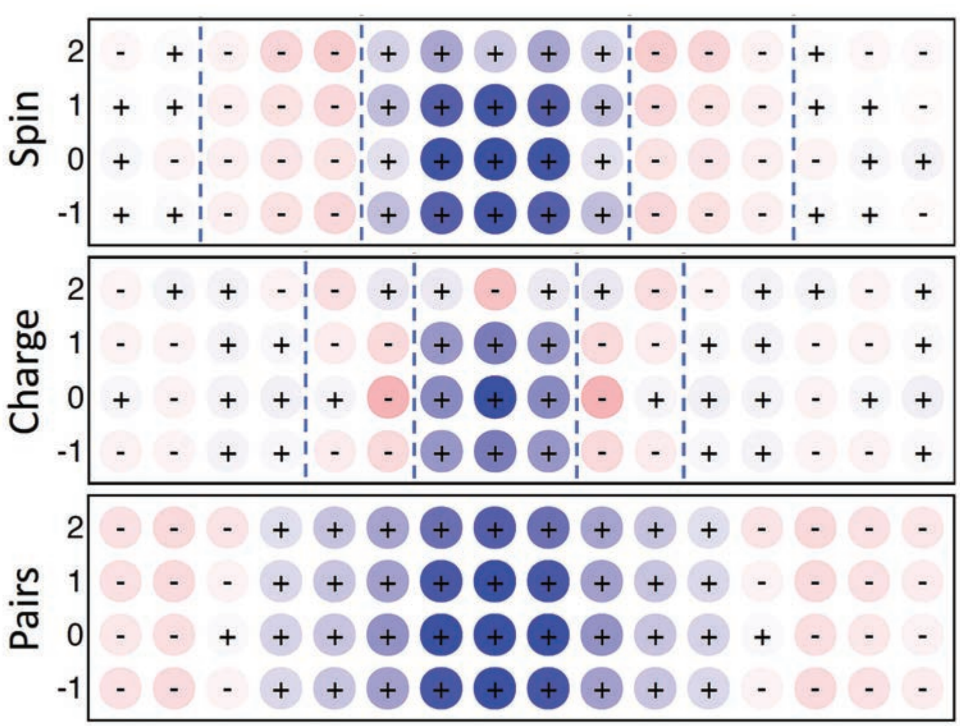
"This is mostly about solving what's now a decades-old problem," said Thomas Maier, an ORNL physicist who led the study with researchers from the University of Tennessee, Knoxville, and the Institute for Theoretical Physics at ETH Zurich. "If we can answer the question of what's the mechanism for superconductivity in certain correlated electron systems and understand the reasons for that behavior, then we can design materials to make the most of that behavior."

Findings appeared in the *Proceedings of the National Academy of Sciences*.

The study used Summit, the Oak Ridge Leadership Computing Facility's 200-petaflop IBM AC922 supercomputing system, to simulate interactions among a system of electrons within a solid. The simulations applied the Hubbard model, which describes a system of interacting electrons in two dimensions, to explore how a class of copper alloys known as cuprates act as superconductors that transmit electricity with no loss of energy.

Cuprates can be used in power transmission and generation but generally display their full superconducting properties under extreme cold — typically hundreds of degrees below freezing. Explaining this behavior could crack the code to deliver superconductivity at room temperature and provide cheap, speedy and sustainable energy.

The Hubbard model, named for British physicist John Hubbard, posits a system of electrons within a 2D lattice. Each electron has a spin — either up or down, similar to the positive and negative poles of a magnet — and no two electrons of the same spin can occupy the same site. The first term of the model describes kinetic energy. In this term, the electrons move, or "hop," back and forth between adjacent sites in the lattice and diagonally between their next nearest neighbors. The second term describes interaction energy and the energy increase when two electrons of opposite spin try to occupy a single site.



An international team of researchers used Summit to model spin, charge and pair density waves in cuprates, a type of copper alloy, to explore the materials' superconducting properties. The results revealed new insights into the relationships between these dynamics as superconductivity develops. Image credit: Thomas Maier, ORNL

Researchers have experimented with layers of copper and oxygen in search of a room-temperature superconductor and adjusted, or “doped,” the Hubbard model over the years to try to understand superconducting properties. The doped models remove electrons, leaving “holes” that encourage the remaining electrons to form pairs that easily conduct electricity.

Under the right conditions, the holes fall in line to form stripes, believed by scientists to compete with superconductivity, and the electrons form a wave pattern, known as a charge and spin density wave. But those models so far fail to reliably explain or predict superconductivity in enough detail for practical use.

“The model in theory would be infinite in size with many distinct phases, which requires extremely large, complex calculations,” Maier said. “We need a simple model that describes all the physics and consistently produces the same results.”

Maier’s team received an allocation grant of 900,000 node-hours on Summit via DOE’s Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, program to explore the model in depth. The results revealed new insights into the relationships between electron spin and charge stripes, including when stripes form as superconductivity develops.

“These were some really heavy computations that couldn’t be done anywhere but on Summit,” Maier said. “We finally had a machine that could support computations for a system large enough to see the stripes. This method allowed us to show that when the stripes show up in charge and spin, the superconducting correlations form a similar wave-like pattern known as a pair density wave. The results could set a new standard for understanding this model.”

Traffic-based building schedules

make smart city even smarter

by Elizabeth Rosenthal
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Using strategically placed traffic sensors, shown as gold spheres, the team assigned vehicle occupants to nearby buildings to estimate their populations and energy consumption. Image credit: Andy Berres, ORNL

The buildings we use and our commutes between them account for more than half of the energy consumed in the United States each year.

To determine how these daily mobility patterns affect energy efficiency and accessibility, researchers at ORNL partnered with the Smart City Division within the City of Chattanooga's Department of Information Technology.

By studying data collected by 45 of Chattanooga's 100 traffic sensors and using computational geometry maps called Voronoi diagrams to pair buildings with nearby intersections, the team created building occupancy schedules that approximate the number of people present in buildings over the course of a year based on estimated vehicle arrival and departure times.

Patterns of commuter behavior compiled in these schedules allow researchers to study a building's energy consumption, which could provide insights needed to design more efficient heating and cooling timetables based on population levels and to enable faster, better informed responses in emergencies.

Led by ORNL researcher Andy Berres, the team studied traffic data to observe intersections and buildings while maintaining the privacy of individuals. The results were published in the journal *Building Simulation*.

"There are a lot of aspects for which the number of people in a building makes a difference, and with these improved occupancy schedules you can get a much more accurate picture of what's actually happening energywise," Berres said.

For example, increases in building occupancy can lead to more demand for heating, ventilation and air conditioning; electricity; and other utilities, whereas decreases in occupancy may result in energy wasted on amenities in unoccupied areas. Although stock occupancy schedules can provide some insights into this balancing act, the team's custom counterparts include more detailed data for individual buildings. The researchers anticipate that tracking monthly and seasonal trends in these schedules will reveal opportunities for enhanced efficiency.

"Basically, we're trying to get a better idea of how many people are where at what times of day," Berres said. "We are currently compiling hourly schedules, but those could be broken up into shorter segments of 5 or 10 or 15 minutes to be more precise."

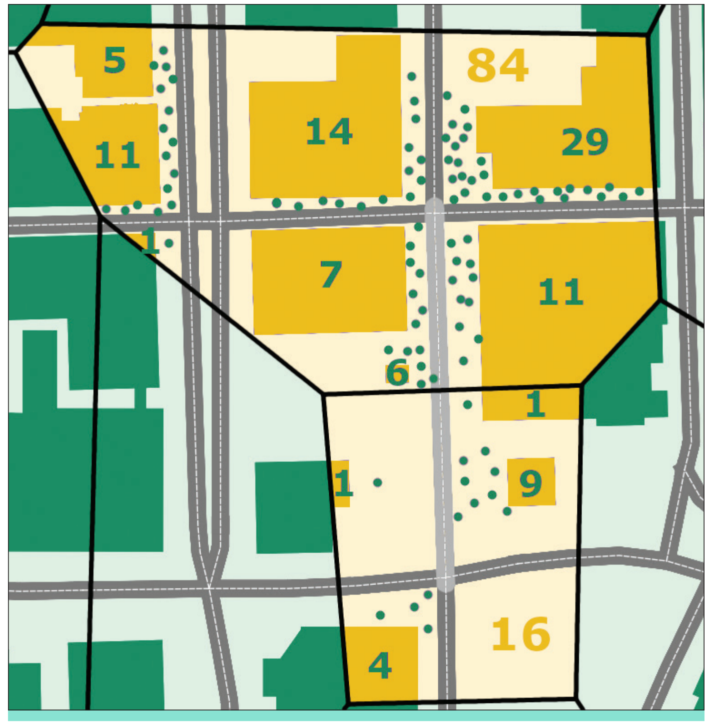
Because traffic and building occupancy decreased during the COVID-19 pandemic — especially in March and April of 2020, when many businesses were closed — Berres compared measured energy use from 2019 provided by EPB of Chattanooga with simulated energy use for both default and custom occupancy levels in 2020. Outside of those two months, weekdays in both years saw similar levels of activity.

Better building occupancy schedules could also help first responders determine how many people in a building may need help evacuating during natural disasters and other emergencies. Between this effort and other ORNL-led "smart city" projects, Berres envisions a future in which daily operations could be adjusted in real time to maximize energy savings in response to traffic incidents.

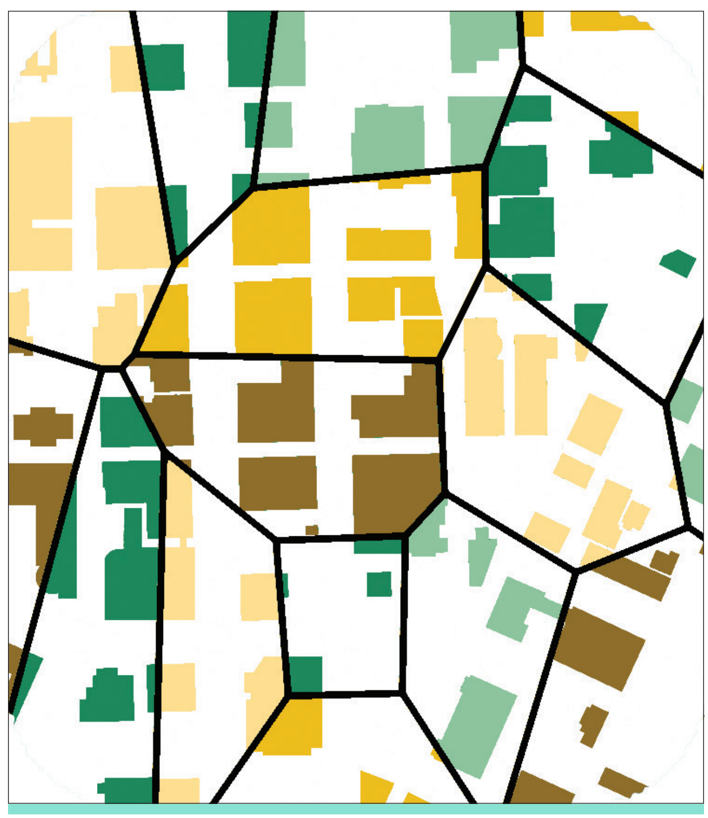
"If there's construction on the interstate, people might come into work later because they didn't account for that amount of traffic," they said. "So, it might be beneficial to start the air conditioning in an office building a little later to save some energy because most people are not there yet."

Updated traffic sensors with the ability to count pedestrians, bicyclists and public transportation users in addition to personal vehicles could further improve the accuracy of building occupancy schedules in Chattanooga and other smart cities, both nationally and internationally.

"Gaining an even better understanding of the time people spend in buildings and adjusting HVAC schedules accordingly could further improve energy efficiency," Berres said.



In the section of the city pictured here, 100 individuals, shown as green spheres, are allocated to buildings adjacent to intersections. Image credit: Andy Berres, ORNL



To easily identify commuter patterns, the team divided Chattanooga into sections, shown here as alternating colors. Better building occupancy schedules for these neighboring areas could eventually improve energy efficiency throughout the entire city. Image credit: Andy Berres, ORNL

Securing our nation

ORNL's National Security Sciences Directorate leverages the lab's translational science capabilities and facilities to solve complex challenges in nuclear, cyber and human security.

Reducing Nuclear Risk

We're advancing the world's understanding of the uranium fuel cycle; designing novel ways to collect and analyze materials; developing new tools to monitor, model, and simulate nuclear operations; and sharing our knowledge with international partners — all to ensure nuclear materials are used only for peaceful purposes.

Securing Critical Assets

ORNL is leading efforts to secure nuclear materials during transport globally; protect supply chains for vital national resources; and develop novel, cost-effective ways to manufacture critical assets domestically — reducing the associated national security risks.

Sensing Planetary Health

Our multidisciplinary science can sense planetary health — and identify changes — in near-real time, delivering critical insights on human populations, the built environment, and critical infrastructures to help mitigate the impacts of climate change, address resource scarcities, and respond to public health crises.

Advancing Human Security

With advances in high-performance computing and geospatial artificial intelligence, we're mapping the built environment, automating feature extraction, and providing vital datasets that help communities recover more quickly from disasters — minimizing the loss of human life.

Creating a Resilient Grid

The energy grid is among our nation's most critical assets. ORNL's researchers are providing real-time situational awareness, enhancing intelligence analysis, and developing technologies to make the grid more resilient against attacks or disruptions.

Advancing Cyber Intelligence

As more components connect to the electric grid — car chargers, smart devices, renewable energy sources — each creates a potential cyberattack point. With novel approaches to identity science and data fusion, we're helping thwart our cyber adversaries to secure the grid of the future.

Image credit: Nathan Armistead, ORNL

COVID-19 research

moves to antiviral drug design

by Jeremy Rumsey
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Developing new drugs that remain potent against emerging variants of COVID-19 is essential to protecting human health and stopping the spread of the highly contagious disease.

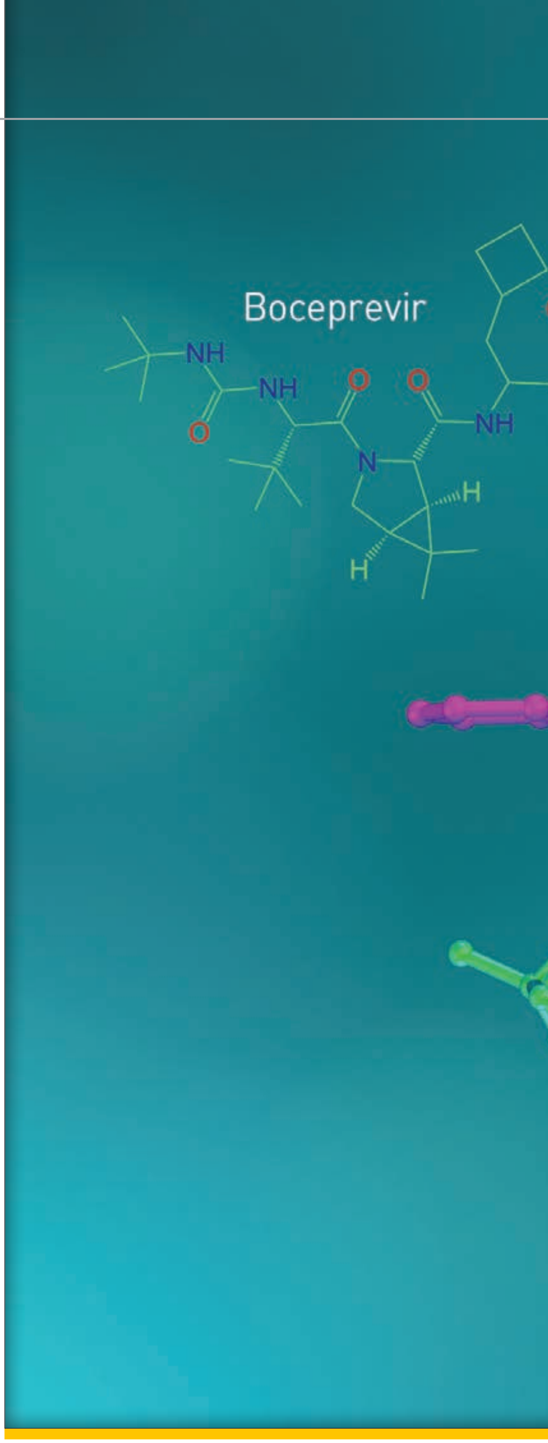
After more than two years of studying SARS-CoV-2 — the virus that causes COVID-19 — ORNL researchers are now designing and testing small-molecule antivirals that block the virus's ability to reproduce. In their most recent study, published in the journal *Nature Communications*, the researchers showed that their antiviral molecules are about as effective as some of the leading drugs on the market today.

The antiviral molecules, called hybrid inhibitors, are made from repurposed drugs used to treat hepatitis C and SARS-CoV — the coronavirus that broke out in 2002.

"From the beginning, our research has revolved around the main protease, which is an enzyme inside SARS-CoV-2 that enables the virus to reproduce. If you shut down the protease, you shut down the virus," said Daniel Kneller, a former ORNL postdoc and the paper's lead author.

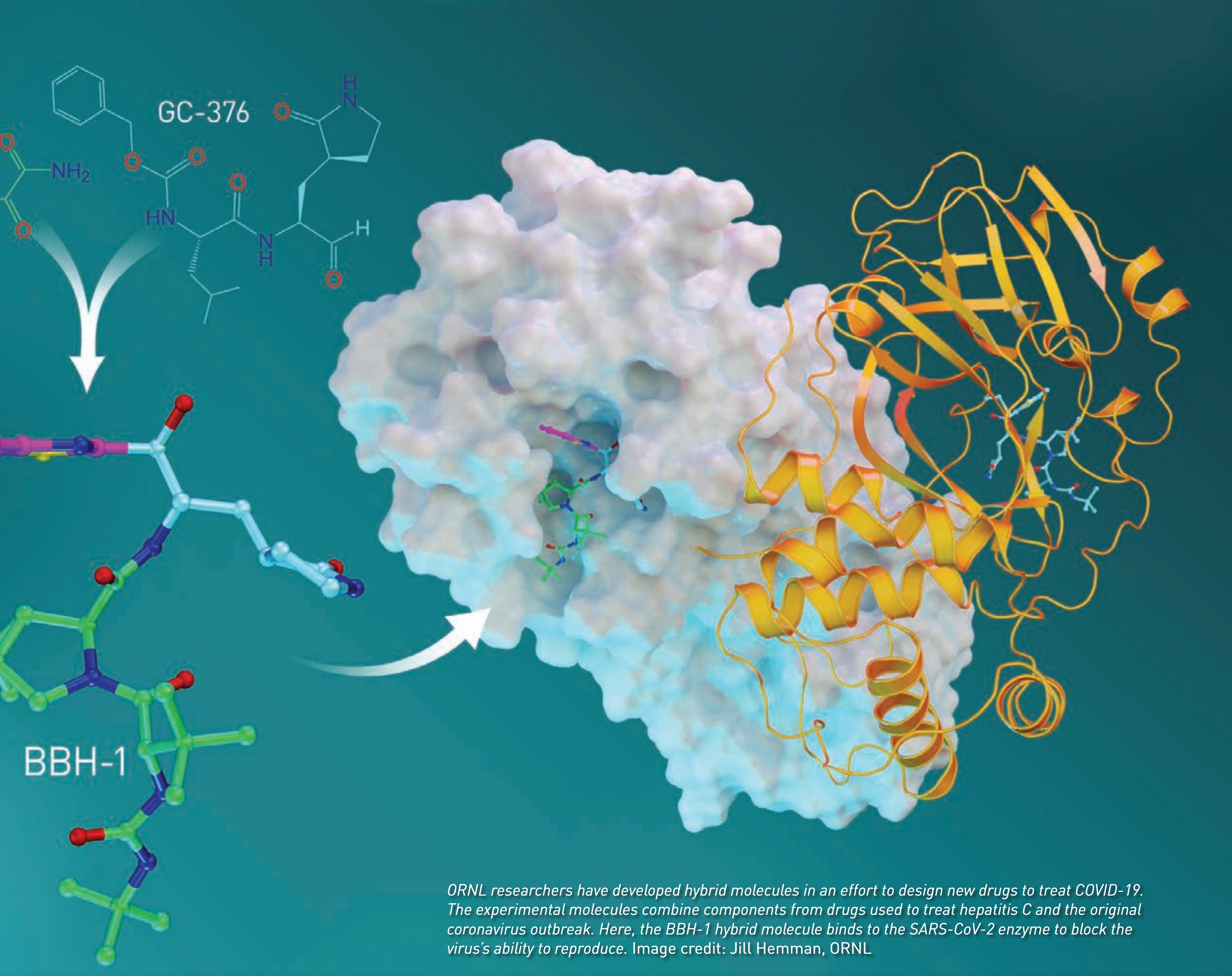
To better understand how the protease works, the researchers used a combination of X-rays and neutron experiments at ORNL's Spallation Neutron Source and High Flux Isotope Reactor to create a comprehensive 3D map of every atom in the protease structure. Next, they charted the vast network of hydrogen bonds that hold the protease together. They also plotted the location of each pocket where the replication process occurs and discovered that the sites are electrically charged.

The team then pivoted to investigating antiviral hepatitis C drugs — boceprevir, narlaprevir and telaprevir — that might be redesigned, or repurposed, to block the SARS-CoV-2 protease.



"This study is the culmination of everything we've learned up to this point. In it, we took the best parts of the hepatitis C drugs and created three new molecules and tested them on SARS-CoV-2's protease," Kneller said.

Each drug molecule has what's called a warhead that links directly to the amino acid site where the natural chemical reaction would occur. Ideally, when the warhead binds to the amino acid site, the resulting combination of the enzyme and the inhibitor should closely represent the natural one.



ORNL researchers have developed hybrid molecules in an effort to design new drugs to treat COVID-19. The experimental molecules combine components from drugs used to treat hepatitis C and the original coronavirus outbreak. Here, the BBH-1 hybrid molecule binds to the SARS-CoV-2 enzyme to block the virus's ability to reproduce. Image credit: Jill Hemman, ORNL

"We found in previous studies that when telaprevir binds, the warhead has a neutral charge and actually faces away from the special amino acid site where interactions would be strong," said ORNL senior scientist Andrey Kovalevsky. "So we designed hybrid inhibitors to provide the exact linkage we needed to establish tight interactions between the inhibitors and the protease."

To expedite measurements of the molecular binding interactions between the three hybrid inhibitors and the SARS-CoV-2 protease, the team used the LADI-DALI beamline at the Institut Laue Langevin nuclear reactor in France. Because neutrons are nondestructive and highly sensitive to light elements such as hydrogen, they provide a powerful tool for studying complex biological processes.

"Neutrons enabled us to see for the first time these very strong binding interactions the hybrid molecules form with the protease," said ILL instrument scientist Matthew Blakeley. "No other experimental technique can provide this level of detail, which is precisely what is needed to truly understand how these molecules work."

The samples used in the experiments were developed at ORNL's Center for Nanophase Materials Sciences and Center for Structural Molecular Biology. Additional experiments performed at the National Institutes of Health also confirmed the neutron results.

"We've shown tremendous ability to apply fundamental knowledge that expedites the timeline to realizing effective treatments," Kovalevsky said. "This is a big step forward not only in fighting COVID-19, but hopefully our research will translate to similar challenges we may face in the future."

Reducing stress:

Neutrons help GE improve 3D-printed parts

by Paul Boisvert
boisvertpl@ornl.gov

The heat, pressure and force that materials experience during manufacturing processes such as forming, casting and molding can cause internal inconsistencies in manufactured metal parts. These inconsistencies include distortions and uneven microstructures, or "strain," which can lead the parts to crack and fail.

Reducing internal strain in manufactured parts is why post-build heat treatments such as annealing are common. Annealing involves heating manufactured parts to high temperatures to decrease internal stress.

GE Global Research scientists are working to improve production models to help better design and heat-treat parts. In a recent study, they focused on parts made using additive manufacturing, where parts are printed layer by layer.

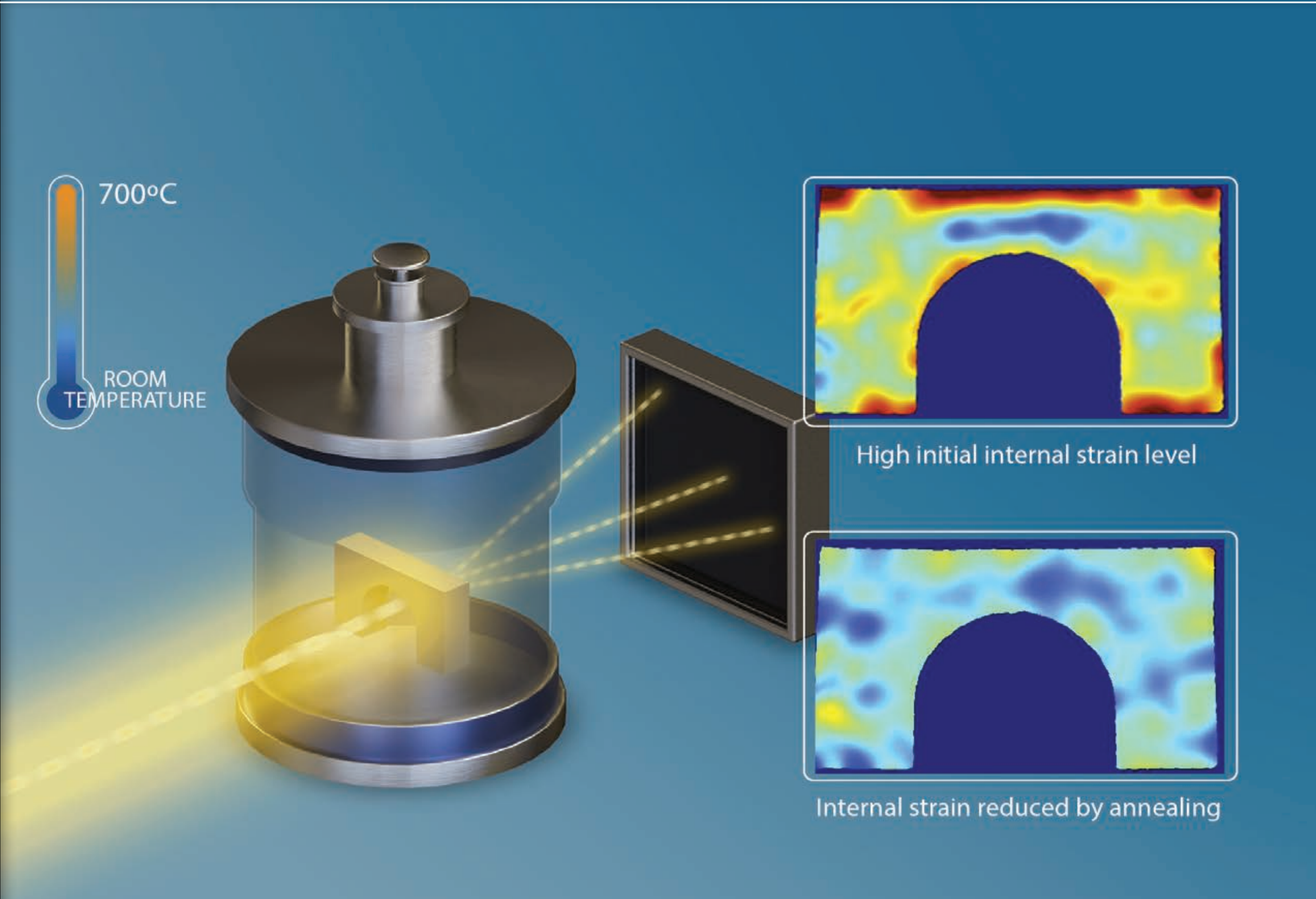
> *"Neutrons helped us look through the furnace walls in real time during the annealing process. We observed where the stress was reduced in the material during heating and at what temperature.*
> — GE Global Research Principal Engineer **Ade Makinde**

Laser-based AM can cause internal strain due to rapid heating and cooling during the process. Annealing can reduce the internal stress, but too much heat can cause unwanted structural changes in the material.

Using neutron diffraction at the VULCAN beamline at ORNL's Spallation Neutron Source, the researchers measured high internal residual strain inside samples of Inconel 625, a common metal alloy. A complementary technique, neutron imaging, was then used at the SNAP beamline to measure — in real time — how annealing the parts reduced the internal strain.

"The amount and distribution of internal strain were related to laser beam speed, laser power and other parameters during production," said Ke An, lead instrument scientist for VULCAN.

"When using laser AM, the top layer being melted is very hot, while the lower layers have cooled. This temperature variation can create internal stresses that can lead to cracking," said Ade Makinde, a principal engineer at GE Global Research. "Neutrons helped us look through the furnace walls in real time during the annealing process. We observed where



GE used neutrons to observe internal strain relief in additively manufactured parts during high-heat processing. The neutrons easily penetrated the vacuum furnace walls and imaged the entire bulk part as the strain was relieved. Image credit: Jill Hemman, ORNL

the stress was reduced in the material during heating and at what temperature.

"It's a balancing act. We need to heat the material, to reduce the stress, but avoid temperatures that are too high, to prevent unwanted structural changes."

The team annealed each 3D-printed part in a vacuum furnace for several hours at either 700 degrees or 875 degrees Celsius. The neutrons easily penetrated the vacuum furnace walls and imaged the entire bulk part as the internal strain was relieved. Stress relief was complete within 1 to 1.5 hours at the lower temperature, while it took only a few minutes at the higher temperature.

The data obtained is helping GE improve its computer modeling of production processes to reduce or eliminate mechanical failures in 3D-printed components. For example, the model can show how changing the shape of a part can make it stronger by minimizing internal stress occurring during production. It can also indicate if changing the width of the laser beam or the speed at which the laser travels can improve production quality.

"ORNL is the only facility in the U.S. with the capability to provide the global neutron user community with complementary diffraction and neutron imaging techniques. We also offer high-speed data acquisition and analytical expertise," said Hassina Bilheux, lead imaging beamline scientist at the High Flux Isotope Reactor. "The VENUS imaging beamline currently under construction at SNS will feature a wider range of neutron energies for users to work with in the future."

"At GE we are extremely happy with the data from these experiments and how easy it was to use the neutron facilities at ORNL," Makinde said. "All the necessary equipment was already installed and calibrated at the beamlines. The furnace at the SNAP beamline maintained controlled temperatures, and everything was synchronized to ensure accurate data acquisition."

Precision machining

produces tiny, light-guiding cubes for advancing info tech

by Dawn Levy
levyd@ornl.gov

Drilling with the beam of a scanning transmission electron microscope, ORNL scientists precisely machined tiny electrically conductive cubes that can interact with light and organized them in patterned structures that confine and relay light's electromagnetic signal. This demonstration is a step toward potentially faster computer chips and more perceptive sensors.

The seeming wizardry of these structures comes from the ability of their surfaces to support collective waves of electrons, called plasmons, with the same frequency as light waves but with much tighter confinement. The light-guiding structures are measured in nanometers, or billionths of a meter — 100,000 times thinner than a human hair.

"These nanoscale cube systems allow extreme confinement of light in specific locations and tunable control of its energy," said ORNL's Kevin Roccapriore. "It's a way to connect signals with very different length scales."

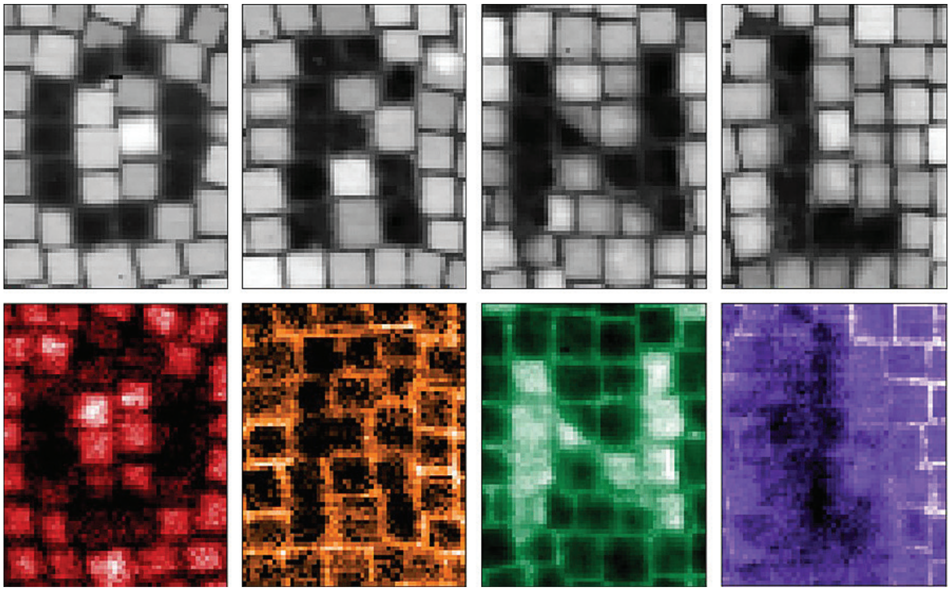
The feat may prove critical for quantum and optical computing. Quantum computers encode information with quantum bits, or qubits, determined by a quantum state of a particle, such as its spin. In optical computers, light — electromagnetic radiation that propagates by massless elementary particles called photons — replaces electrons as the messenger.

"Light is the preferred way to communicate with qubits, but you cannot connect contacts to them directly," said Sergei Kalinin, formerly of ORNL. "The problem with visible light is its wavelengths range from about 380 nanometers for violet to around 700 nanometers for red. That's too big because we want to make devices only a few nanometers in size." This work aims to create a framework to move technology beyond classical electronics and Moore's law, an observation that transistors shrink as technology advances.

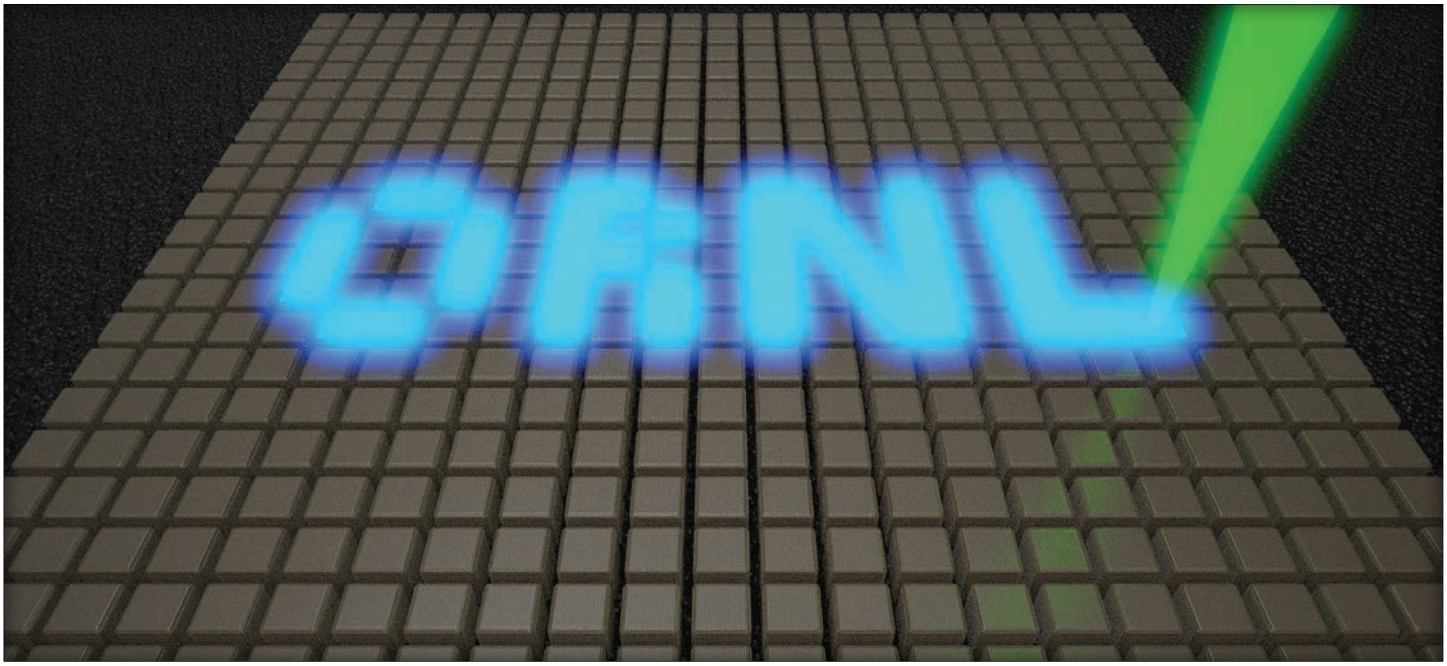
"If you try to put 'light' and 'small' together, that's exactly where plasmonics comes into play," Kalinin added.

The ORNL-led achievement may help overcome a signal size mismatch that threatens the integration of components made of different materials. Those components will need to communicate with each other in next-generation optoelectronic devices.

The team used cubes made of a transparent semiconductor. The fact that the cube is a semiconductor is essential to its energy tunability. The energy of a light wave is related to its frequency. Wavelengths of visible light appear to the human eye as colors. Because a semiconductor can



ORNL scientists used an electron beam for precision machining of nanoscale materials. Cubes were milled to change their shape and could also be removed from an array. Image credit: Kevin Roccapriore, ORNL

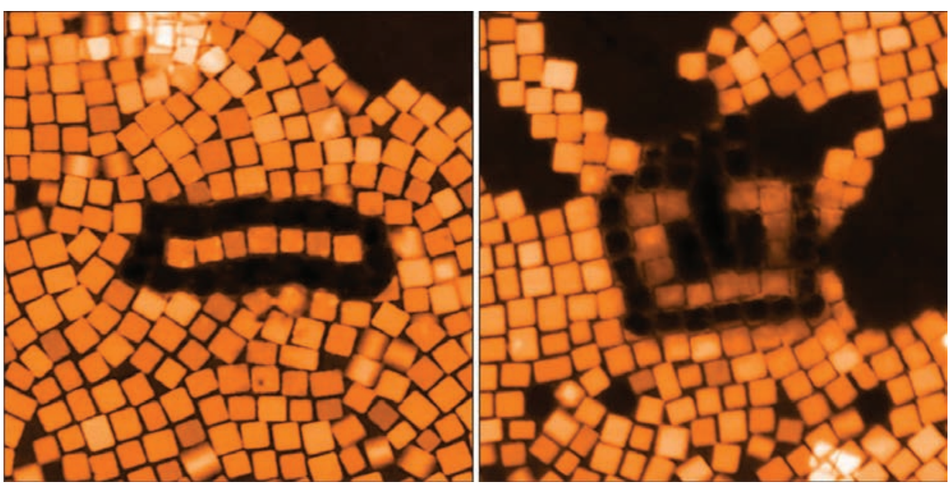


An electron beam imparts energy that moves or sculpts building blocks in an array. The designer blocks guide undulating clouds of electrons called plasmons. Image credit: Kevin Roccapriore, ORNL

be doped — that is, a small impurity can be added — its wavelength can be shifted on the spectrum.

Synthesized at the University of Texas at Austin, the cubes were each 10 nanometers wide, which is much smaller than the wavelength of visible light. They self-assembled, evenly spaced apart on a substrate, creating 2D arrays that were sent to ORNL.

"That the cubes do not directly touch is important for the collective behavior," said Roccapriore. "Each cube individually has its own plasmon behavior. When we bring them together in geometries like a nanowire, they talk to one another and produce new effects that are not typically seen in similar geometries that aren't made up of individual elements." Shifting the electron beam current from imaging to modification mode, Roccapriore removed entire cubes from an array as well as bits of cubes and even select chemical elements.



Each cube shown has its own plasmonic behavior. Bring them together in patterns — an antenna, left image, or split ring resonator, right image — and they "talk," producing unique effects. Image credit: Kevin Roccapriore, ORNL

The key to characterizing plasmonic behavior within single cubes and among collective cube assemblies was electron energy loss spectroscopy. It uses a scanning transmission electron microscope with an electron beam filtered to energies within a narrow range. The beam loses energy as its electrons pass through the sample, interact with electrons in the material, and transfer a little energy to the system by exciting plasmons.

"Electron energy loss spectroscopy provides deep insights into exotic physics and quantum phenomena related to plasmonic behavior," said Scanning Transmission Electron Microscopy Group Leader Andrew Lupini, who helped map the energies of electrons in the cubes and arrays of cubes. "This technique lets us analyze evolving plasmonic responses in real time as the cubes are sculpted. We can figure out relationships between arrangements of cubes and their plasmonic properties."

This new knowledge will provide the foundational understanding needed to eventually mass-produce structures that can direct the flow of light in plasmonic nanocircuits.

For more information: https://www.ornl.gov/news/precision-machining-produces-tiny-light-guiding-cubes-advancing-info-tech

Polymer gives 3D-printed sand super strength

by Ashley Huff
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ORNL researchers have designed a novel polymer to bind and strengthen silica sand for binder jet additive manufacturing, a 3D-printing method used by industries for prototyping and parts production.

The printable polymer enables sand structures with intricate geometries and exceptional strength; it is also water soluble.

In a study published in *Nature Communications*, the team demonstrates a 3D-printed sand bridge that at 6.5 centimeters can hold 300 times its own weight, a feat analogous to 12 Empire State Buildings sitting on the Brooklyn Bridge.

The binder jet printing process is cheaper and faster than other 3D-printing methods used by industry and makes it possible to create 3D structures from a variety of powdered materials, offering advantages in cost and scalability. The concept stems from inkjet printing, but instead of using ink, the printer head jets out a liquid polymer to bind a powdered material, such as sand, building up a 3D design layer by layer. The binding polymer is what gives the printed sand its strength.

A novel polymer developed at ORNL strengthens sand for additive manufacturing applications. A 6.5 centimeter 3D-printed sand bridge, shown here, held 300 times its own weight. Image credit: Dustin Gilmer, University of Tennessee, Knoxville

The team used polymer expertise to tailor a polyethyleneimine, or PEI, binder that doubled the strength of sand parts compared with conventional binders.

Parts printed via binder jetting are initially porous when removed from the print bed. They can be strengthened by infiltrating the design with an additional super-glue material called cyanoacrylate that fills in the gaps. In the study, this second step provided an eightfold strength increase on top of the first step, making a polymer sand composite stronger than any other and any known building materials, including masonry.

"Few polymers are suited to serve as a binder for this application. We were looking for specific properties, such as solubility, that would give us the best result. Our key finding was in the unique molecular structure of our PEI binder that makes it reactive with cyanoacrylate to achieve exceptional strength," said ORNL's Tomonori Saito, a lead researcher on the project.

Parts formed with conventional binders are made denser with infiltrate materials such as super glue, but none have come close to the performance of the PEI binder. The PEI binder's impressive strength stems from the way the polymer reacts to bond with cyanoacrylate during curing.

One potential application for the super-strength sand is to advance 3D-printed sand cores, or "tools," for composites manufacturing.

Silica sand is a cheap, readily available material that has been gaining interest in automotive and aerospace sectors for creating composite parts. Lightweight materials such as carbon fiber or fiberglass are wrapped around the tools and cured with heat. Silica sand is attractive for tooling because it does not change dimensions when heated and because it offers a unique advantage in washable tooling. In composite applications, using a water-soluble binder to form sand tools is significant because it enables a simple washout step with tap water to remove the sand, leaving a hollow composite form.

"To ensure accuracy in tooling parts, you need a material that does not change shape during the process, which is why silica sand has been promising. The challenge has been to overcome structural weakness in sand parts," said Dustin Gilmer, a University of Tennessee Bredesen Center student and the study's lead author.

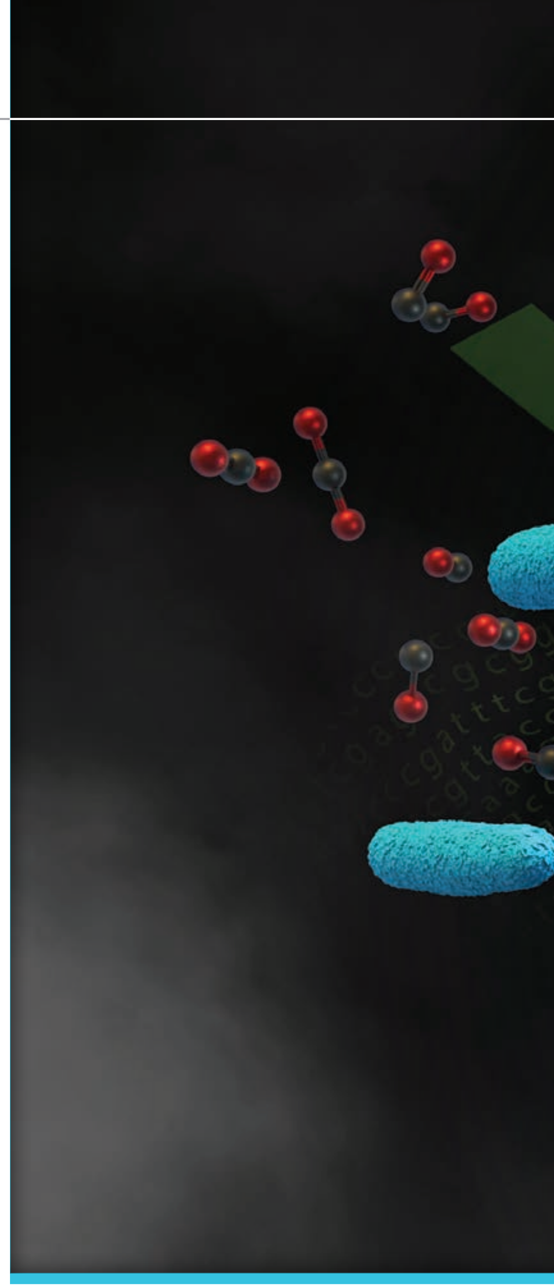
Current sand casting molds and cores have limited industrial use because commercial methods, such as washout tooling, apply heat and pressure that can cause sand parts to break or fail on the first try. Stronger sand parts are needed to support manufacturing at a large scale and enable rapid part production.

"Our high-strength polymer sand composite elevates the complexity of parts that can be made with binder jetting methods, enabling more intricate geometries, and widens applications for manufacturing, tooling and construction," Gilmer said.

ORNL scientist Tomonori Saito shows a 3D-printed sandcastle at the DOE Manufacturing Demonstration Facility at ORNL. Image credit: Carlos Jones, ORNL

Microbes turn waste gases

into valuable chemicals



by Kim Askey
askeyka@ornl.gov

A team of scientists from LanzaTech, Northwestern University and ORNL have engineered microorganisms to turn emissions from industrial processes into acetone and isopropanol, or IPA. These widely used chemicals serve as the basis of thousands of products, from fuels and solvents to acrylic glass and fabrics.

> "Synthetic biology can be a powerful tool in the quest to advance decarbonization and address climate change. Our scientists leverage world-class capabilities, working closely with industry to harness biological systems to produce valuable fuels and chemicals that support a thriving national bioeconomy.
>
> — ORNL Associate Laboratory Director **Stan Wullschleger**

The technology uses microbes called *Clostridium autoethanogenum*, or *C. auto*, as tiny-but-powerful factories that convert carbon from agricultural, industrial and societal waste streams into useful chemicals. The process recycles carbon that would otherwise be released as greenhouse gases that accelerate climate change.

In the race to net-zero emissions, this platform provides a step toward a circular carbon economy that can replace products made from fossil resources.

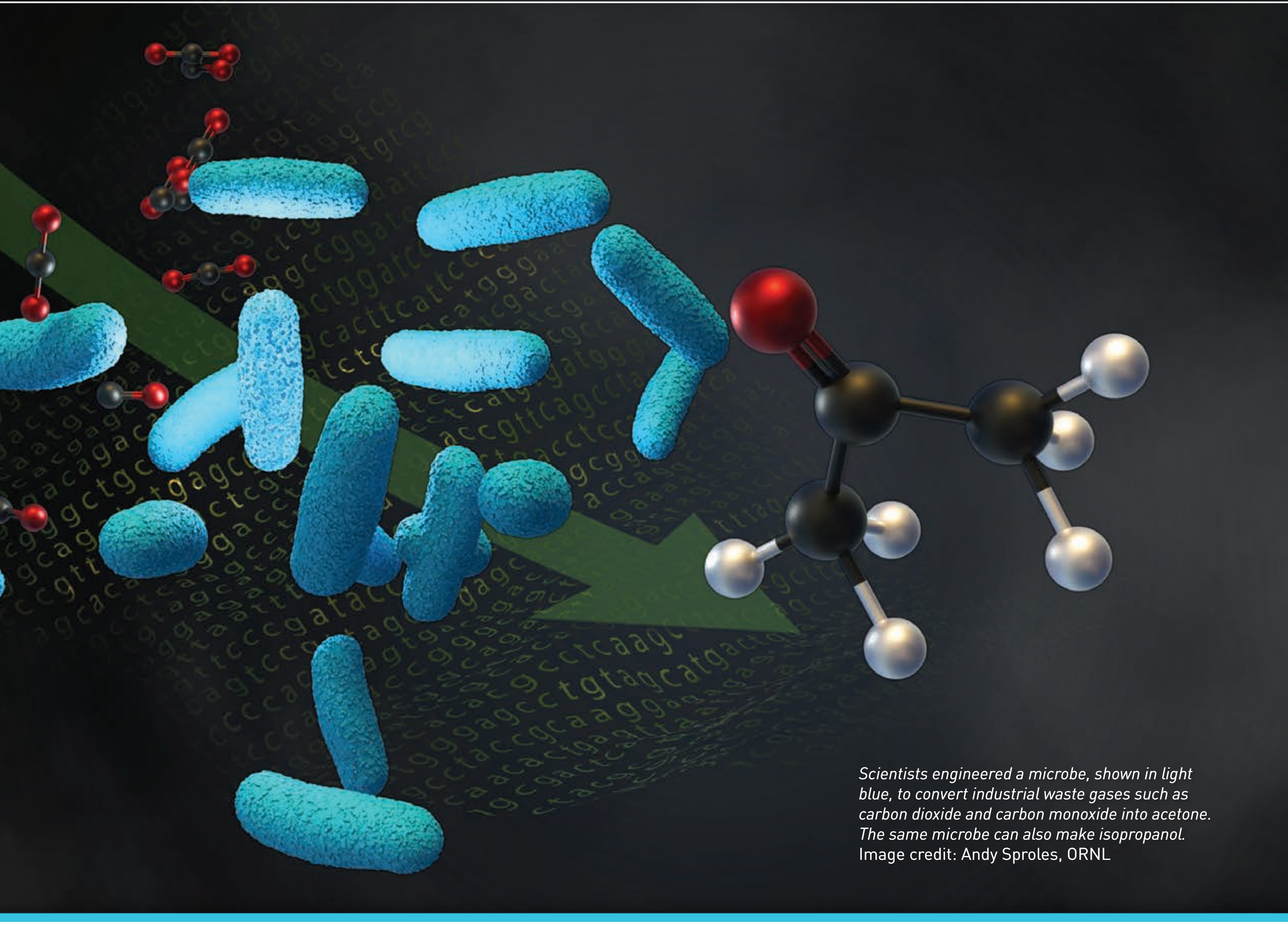
"This bioprocess provides a sustainable alternative to today's production routes to these essential chemicals, which currently rely on fresh fossil feedstocks and result in significant toxic waste," said Jennifer Holmgren, CEO of LanzaTech.

"We can reduce greenhouse gases by more than 160 percent, achieve carbon-negative production and lock up carbon that would have ended up in the atmosphere."

LanzaTech is scaling up this technology, which can be inserted into their existing systems and deployed for use around the world.

"Synthetic biology can be a powerful tool in the quest to advance decarbonization and address climate change," said ORNL Associate Laboratory Director Stan Wullschleger. "Our scientists leverage world-class capabilities, working closely with industry to harness biological systems to produce valuable fuels and chemicals that support a thriving national bioeconomy."

The research began at LanzaTech, where scientists previously commercialized a process using *C. auto* strains that produces ethanol, a common biofuel, from carbon emissions. Identifying the best enzymes for acetone and IPA produc-



Scientists engineered a microbe, shown in light blue, to convert industrial waste gases such as carbon dioxide and carbon monoxide into acetone. The same microbe can also make isopropanol. Image credit: Andy Sproles, ORNL

tion and engineering microbial strains to achieve efficient, high-yielding carbon-to-chemical conversion presented a complex scientific challenge.

The scientists used a three-pronged approach that comprised innovations in pathway screening, strain optimization and process development. As a first step, LanzaTech screened nearly 300 strains for enzymes that could be useful in the acetone- and IPA-producing pathways.

Further optimization relied on cutting-edge synthetic biology tools, including cell-free prototyping by Northwestern University, advanced modeling by LanzaTech and molecular analyses by ORNL.

"Oak Ridge has very unique capabilities in terms of DNA sequencing, systems biology and various metabolomics and proteomics," Michael Köpke, LanzaTech's vice president for synthetic biology, said. "ORNL's expertise helped us troubleshoot the process to find out which steps may be limiting."

Proteomics, the study of proteins, and metabolomics, the study of small molecules called metabolites, provide a molecular-level view of which specific chemicals are being used and produced by a microbe. Like any organism, when microbes consume or metabolize the substances they need to survive, they produce byproducts. For scientists engineering microbes to produce certain substances, these byproducts represent bottlenecks.

"The protein and metabolite profiles show where a production bottleneck is occurring inside the *C. auto* cell," said Tim Tschaplinski, head of ORNL's Biodesign and Systems Biology Section. "We can see what needs to be modified next in the pathways to flow more of the carbon to the product."

The optimization process was enabled by ORNL's holistic systems biology approach, which gives scientists a more comprehensive view of what's happening in the cell, Tschaplinski said. "We use one 'omic' to confirm another. By looking at the system as a whole, we can explore different avenues to enhance the generation of the desired product."

"We found one of the enzymes, in particular, gave a significant boost once we increased production," Köpke said. "And we found that through a lot of systems biology and proteomics analyses that were done by Oak Ridge."

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.

Duncan Moseley

Postdoc, Materials Science and Technology Division
Ph.D., Inorganic Chemistry, University of Tennessee, Knoxville
Hometown: Austin, Texas

What are you working on at ORNL?

I primarily use neutron scattering and diffraction techniques to study hybrid lattice and spin excitations in various materials. My work will allow us to discover how strong coupling between lattice vibrations, electrons and spins can promote the discovery of quantum and energy materials with novel properties.

What would you like to do in your career?

Since beginning my postdoc here, I have really developed a fascination with neutron scattering. I would like to continue using these techniques to study a variety of interesting materials in a national laboratory environment such as ORNL, either as an instrument or staff scientist.

Why did you choose a career in science?

I've had a knack for science since I was young. I have found that I love to learn new ideas and how things work. I particularly enjoy the hands-on technical work and problem-solving aspects of science. Making new discoveries and analyzing experimental data is right up my alley.

Dipti Kamath

Postdoc, Manufacturing Science Division
Ph.D., Environmental Engineering, Michigan State University
Hometown: Thrissur, India

What are you working on at ORNL?

I work on the technoeconomic and life cycle assessment of integrated biorefinery technologies for paper and pulp industries, additive manufacturing and biomass allocation optimization. In addition, I also serve as a technical account manager for DOE's Better Plants program.

What would you like to do in your career?

My career goals focus on manufacturing sustainability, by focusing on energy efficiency and circular economy. I want to use my expertise in technoeconomic and life cycle assessment to evaluate the unintended consequences of various technologies and help decarbonize the manufacturing sector.

Why did you choose a career in science?

Science has allowed me to indulge in my fascination for the world around us. Science classes were always fun, especially the problem-solving part. A career in science means I can keep solving problems like the ones I've worked on all my life.

Zening (Zach) Liu

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Chemistry, Auburn University
Hometown: Chengdu, Sichuan Province, China

What are you working on at ORNL?

My research focuses on understanding the behaviors of soft materials at interface and in solution at the molecular level. The findings provide significant insights into the functioning of soft material aggregates, envisioned in next-generation computational systems, 3D-printing media, antibiotics and ion conducting materials.

What would you like to do in your career?

I love doing research and love solving chemistry puzzles. I would like to continue working in material sciences to not only explore materials but to also deliver practical solutions to real-world challenges.

Why did you choose a career in science?

My childhood dream — to explain the wonders of nature — guided me to become a chemist. I immensely enjoy working in chemistry labs, where I have the chance to address fundamental questions in scientific ways and create intriguing results.

Michelle Lehmann

Graduate student, Chemical Sciences Division
Ph.D. student, Polymer Chemistry, University of Tennessee, Knoxville
Hometown: Bairnsdale, Victoria, Australia

What are you working on at ORNL?

I am working on polymer electrolytes and ion-exchange membranes for fuel cells and large-scale batteries. My research involves designing and synthesizing polymers with improved stability and performance.

What would you like to do in your career?

I would like to stay in research, working on next-generation electrochemical conversion and storage technologies. I hope to aid in the advancement of technologies to support decarbonization of the electricity and transportation sectors.

Why did you choose a career in science?

I chose a career in chemistry because I really enjoyed my undergraduate chemistry classes. Participating in undergraduate research led me to my interest in polymer chemistry and ion-exchange membranes. A career in science allows me to evolve and learn continually and make a positive impact on the world.

Damilola Olayinka Akamo

Graduate student, Buildings and Transportation Science Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville
Hometown: Abeokuta, Nigeria

What are you working on at ORNL?

My research focuses on the synthesis, development and characterization of salt hydrate–based phase change materials. These materials can serve as a thermal battery, storing and releasing thermal energy through phase change. They are part of the next-generation energy storage technologies for the decarbonization of our entire energy system.

What would you like to do in your career?

I would like to contribute to the effort to address global energy concerns by discovering and characterizing novel materials for renewable energy applications. My goal is to have a better understanding of processing–structure–property relationships and the performance of these innovative materials in energy systems and other applications.

Why did you choose a career in science?

My interest and passion for science stem from my curiosity about the world around me. Also, close relatives with scientific backgrounds influenced my scientific career choice. Science allows me to think critically and find answers to complex problems for the benefit of humanity, which I find rewarding.

Alexandra Kahl

Graduate student, Geospatial Science and Human Security Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville
Hometown: Mount Jackson, Virginia

What are you working on at ORNL?

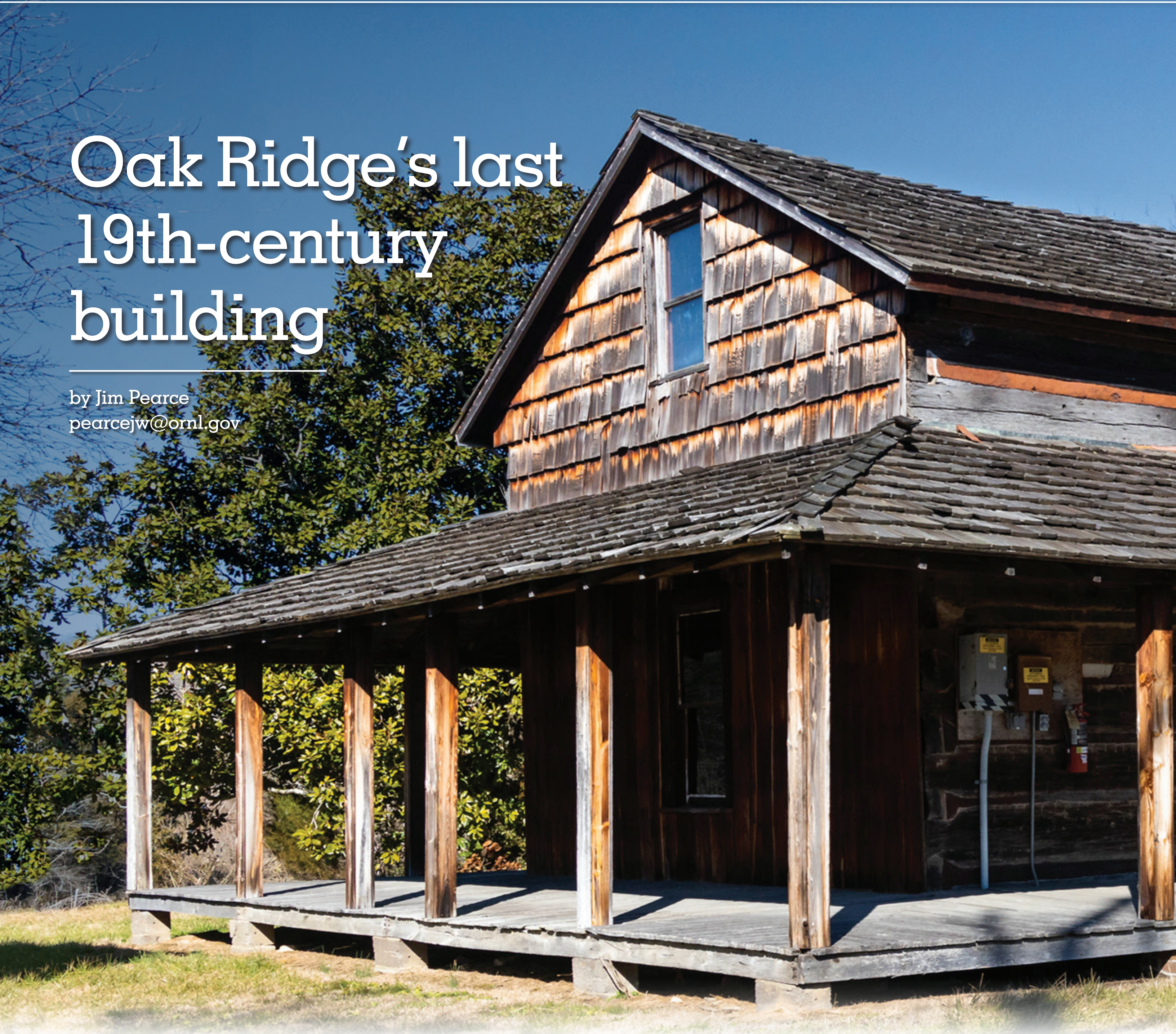
My research is focused on the impacts of winter storms and long-term outages on the U.S. electric grid and vulnerable populations.

What would you like to do in your career?

After finishing my Ph.D., I am interested in pursuing a full-time research position at a national lab or working with our DOE partners in Washington, D.C. Regardless of my specific position, I hope I can continue to work on resilience-related problems and make a contribution to mitigating and adapting to climate change.

Why did you choose a career in science?

I chose this path because it gives me the opportunity to work on problems that I care about and use my creative side to develop new solutions.



Oak Ridge's last 19th-century building

by Jim Pearce
pearcejw@ornl.gov

ORNL and the "secret city" of Oak Ridge, Tennessee, were built in a hurry in the early 1940s in a sparsely populated region of East Tennessee as part of World War II's Manhattan Project.

At the time, there were four small settlements in the area — Scarborough, Robertsville, Wheat and Elza. Many homes in these agricultural communities were removed as construction progressed, and most of the rest were demolished after the war to make room for new development. So, you might not expect to find a 200-year-old log cabin in the neighborhood today.

Nevertheless, about a mile from the laboratory's boundary, Freels Bend Cabin sits atop a rise overlooking Melton Hill Lake. Edward Freels is credited with building the oldest portion of the cabin in about 1810. The Freels family had arrived in East Tennessee from North Carolina in the 1790s and farmed several hundred acres in the area, raising corn and cattle.

When the cabin was built, not far from Scarborough, the homestead looked out over fields leading down to the Clinch River. It gained a lakeside view only after the Tennessee Valley Authority dammed the river in the early 1960s, an act that almost, but not quite, inundated the structure. That was just the latest example of the cabin's knack for survival.

When the government purchased the surrounding farmland in 1942, the cabin was preserved as part of a picnic area for Manhattan

Image credit: Carlos Jones, ORNL

Project staff, and it continues to be used for recreational purposes and as an educational center for local schools and ORNL.

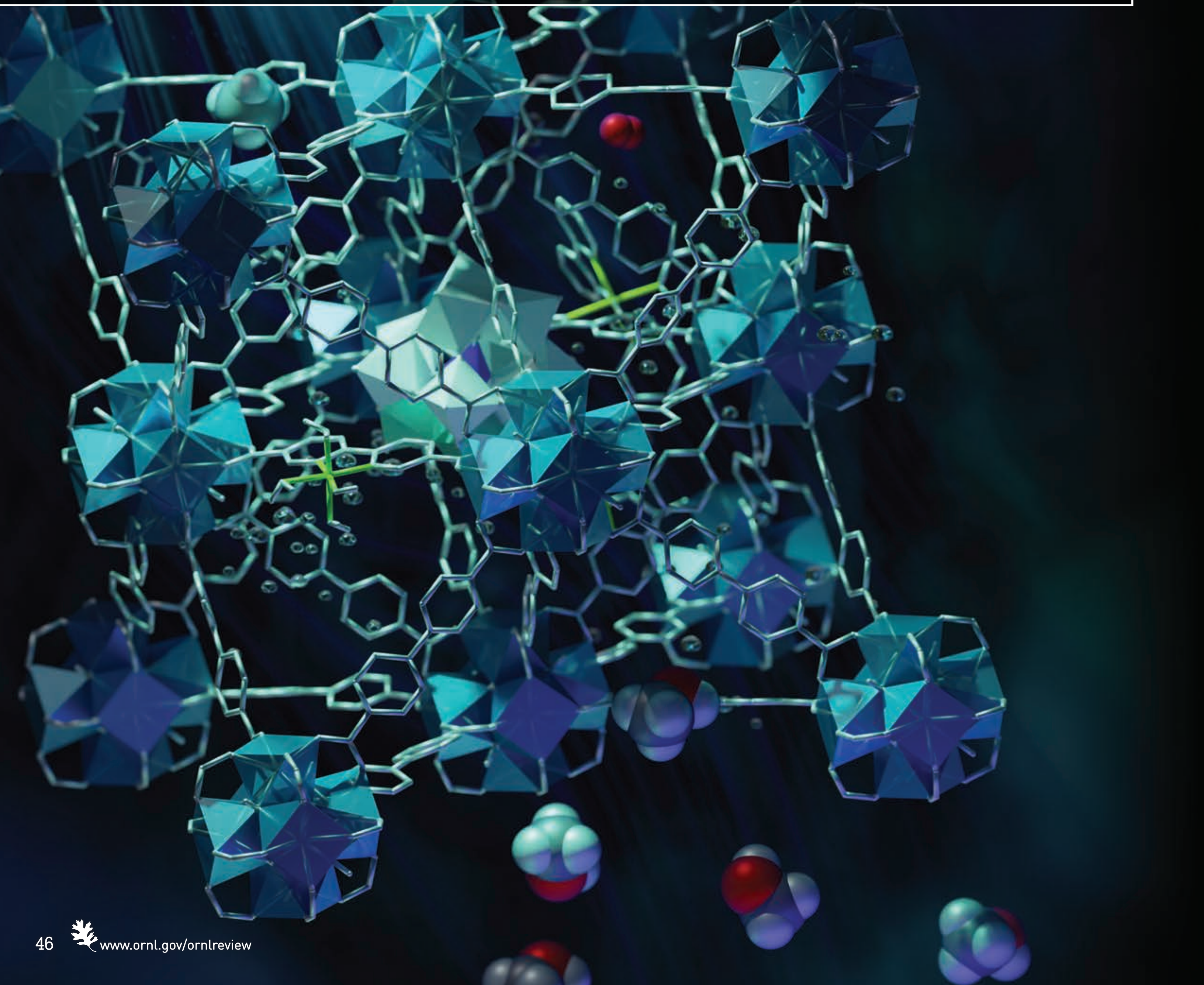
The cabin consists of two large rooms — the one that Edward Freels built in 1810, which has a loft that is reached by a ladder, and another added in 1844. The rooms share a large, limestone chimney, also added in 1844. This arrangement — two rooms on either side of a chimney — is known as a "saddlebag" cabin for its resemblance to a saddlebag that hangs over either side of a horse.

New windows and doors were added around 1900. In the late 1940s, the Atomic Energy Commission replaced the mud chinking between the logs with concrete and built a covered porch that wraps all four sides of the cabin to make it more suitable as a recreation venue.

The cabin is the only remaining 19th-century dwelling in Oak Ridge and was added to the National Register of Historic Places in 1992.

Visiting the rustic cabin today, in a secluded corner of the DOE's Oak Ridge Reservation, it's easy to imagine that it's still the early 1940s. It's harder to fathom the scale of the transformation that the Manhattan Project brought to the region, to the world, and, particularly, to the lives of the residents of four small farming communities, as they were relocated to make way for the enormous scientific and industrial undertaking that ushered in the nuclear age.

Welcome to Research Insights



Toward a Carbon Neutral Future, Part I: Novel research for shrinking the carbon footprint

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

This issue highlights recent advances by ORNL staff to support the United States' ambitious and achievable goal to reduce net greenhouse gas (GHG) emissions by 2030. Achieving the nation's 2030 GHG goals will place the United States firmly on a path to reach net zero by 2050.

In recent years, ORNL has developed a substantial fundamental and applied research program as part of our *Transformational Decarbonization Initiative*. Articles in this issue showcase ORNL GHG emissions reduction projects with a diverse set of applications. In pursuit of sustainable climate mitigation strategies, these articles highlight (1) development of a new class of CO_2 direct air-capture adsorbents, (2) creation of designer cement mixtures that reduce CO_2 emissions from building materials, (3) optimization of plant traits for bioenergy and soil carbon storage, (4) analysis of biomass resources along with development and implementation of next-generation modeling tools to more accurately assess resource allocation options for biomass-to-end-use supply chains, and (5) identification of novel biomass supplies and policy bottlenecks that affect our ability to harness feedstocks for bioenergy with carbon capture and storage.

The articles highlighted in this issue of *Research Insights* represent a small fraction of the ORNL research portfolio dedicated to support the nation's net-zero emission goals. We hope that you enjoy the sampling of the exceptional work being performed by the ORNL research community.

Reducing Atmospheric Carbon Dioxide through Direct Air Capture

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INTRODUCTION

Climate change can be attributed primarily to human activities that began with the Industrial Revolution. These activities have led to accelerated greenhouse gas emissions. In particular, the atmospheric CO_2 concentration, which is currently about 416 ppm, is higher than at any time in at least 2 million years. Cumulative anthropogenic CO_2 emissions are strongly correlated to the measured increase in global surface temperature. Notably, the only remaining scenarios that could limit the total temperature increase to less than 2°C by the end of the century require carbon emissions to fall to essentially zero during the next couple of decades. This decline would need to be followed by gigaton-scale deployment of negative emissions technologies (NETs) to remove CO_2 from the atmosphere, and the CO_2 would need to be stored permanently in designated geological reservoirs [1].

Over the past two decades, technologies that capture CO_2 from the atmosphere, or direct air capture (DAC), have been developed to mitigate climate change [2]. Other NETs include afforestation/reforestation, mineralization, and bioenergy with carbon capture and sequestration. These options may be very slow, can be constrained by land availability, and could present threats to biodiversity and food security. In direct contrast, DAC technologies have a relatively small footprint, boast flexibility of placement, and have a high CO_2 removal rate and capacity. Once CO_2 is captured, it can be transported through pipelines and injected underground for permanent sequestration in geological reservoirs, or it can be supplied to industries that use it or convert it into useful products. If DAC technologies are scaled up and deployed worldwide, they could remove billions of tons of CO_2 from the atmosphere per year. However, to be sustainable and economically viable, these technologies must be energy efficient, should employ renewable or low-carbon energy sources, and must cost less than \$100/ton of captured CO_2. Despite significant progress, DAC technologies are still considered underdeveloped and are not ready to make a substantial impact on climate change.

Over the past 6 years, Oak Ridge National Laboratory (ORNL) has developed new materials and processes for energy-efficient, sustainable DAC technology. This article focuses on ORNL's recent DAC technology efforts, starting with the initial discovery, continuing with basic and applied research, and ultimately leading to a DAC technology that is ready for commercialization [3].

BACKGROUND

State-of-the-art DAC technologies based on aqueous alkaline solvents (e.g., NaOH, KOH) or solid-supported amines developed over the past decade have high energy requirements, on the order of 4–12 GJ/ton CO_2, and relatively high costs of ~\$100–\$600/ton CO_2 [2]. Two pioneering companies have been developing DAC technologies based on these approaches. Carbon Engineering (https://carbonengineering.com/), based in Canada, currently captures CO_2 from air using an aqueous KOH solvent at a scale of 1 ton CO_2/day, with plans to scale up to 1 million tons CO_2/year. The main limitation of this technology is the very high temperatures, ~900°C, required for solvent regeneration. Climeworks (https://climeworks.com/), based in Switzerland, employs a solid-supported amine sorbent for DAC to capture 4,000 tons CO_2/year, which is liquified and injected underground for long-term storage through mineralization. However, the sorbent materials employed are relatively expensive and tend to chemically degrade after a few capture-and-release cycles.

Our team in the Chemical Separations Group at ORNL recently discovered a new class of CO_2 absorbents known as bis-iminoguanidines (BIGs), which are readily accessible by imine condensation of aminoguanidinium salts with di-aldehydes or di-ketones [4]. When BIGs are dissolved in water, they produce alkaline solutions that react with the CO_2 from air and form an insoluble carbonate salt. After the crystalline salt is filtered from the solution, it is heated at relatively low temperatures (80°C–120°C) to release the CO_2 and regenerate the BIG sorbent (Figure 1A). Unfortunately, the CO_2 capacity and rate at which it is absorbed by BIGs can be low, especially from air. Therefore, the process must be modified to increase the amount of CO_2 captured

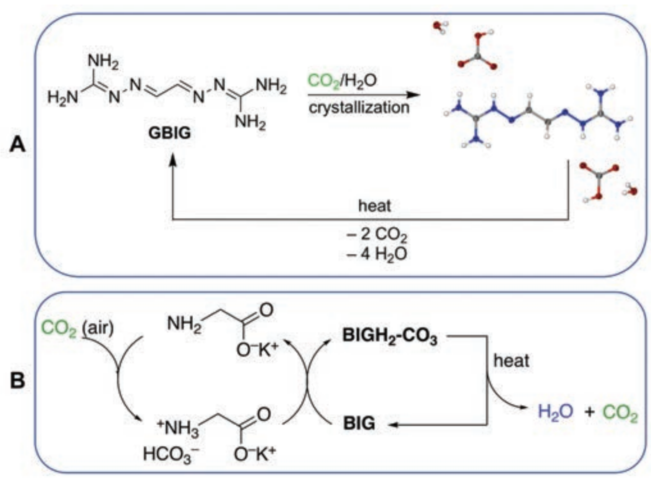

Figure 1. DAC with BIGs: (A) CO_2 capture with the prototype glyoxal-bis-iminoguanidine, forming a crystalline bicarbonate salt of low aqueous solubility (x-ray crystal structure shown at right) [7]; (B) two-cycle DAC by fast absorption with amino acids such as glycine (shown at left) and carbonate crystallization with BIGs (shown at right) [8].

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and to speed up CO_2 absorption. To address these limitations, we considered a two-cycle approach that combines aqueous amino acids [5] or small peptides [6] with BIG compounds as the sorbent mixture (Figure 1B). That is, amino acids are involved in the absorption cycle, and BIGs are involved in the regeneration cycle. Amino acids and peptides are the building blocks of proteins, so they have lower toxicity and volatility than amines, the sorbents currently used in industrial CO_2 capture.

RESULTS

CO_2 removal with BIGs. An aqueous solution of the prototype BIG compound, glyoxal-bis-iminoguanidine (GBIG) reacts with CO_2 to form a crystalline bicarbonate salt with relatively low aqueous solubility [7]. The GBIG bicarbonate crystals can be filtered easily from the solution and heated at relatively mild temperatures (80°C–120°C) to release the CO_2 and regenerate the GBIG compound. The CO_2 capture cycle with GBIG was tested with a flue gas simulant (13% CO_2), resulting in a CO_2 crystallization yield of 89% and quantitative GBIG regeneration, both of which were sustained for 10 consecutive cycles (Figure 2). The 151.5 kJ/mol CO_2 measured regeneration energy of GBIG is 24% lower than the regeneration energy of aqueous monoethanolamine, a benchmark industrial CO_2 solvent for which excessive energy is consumed in heating and vaporization of water [7].

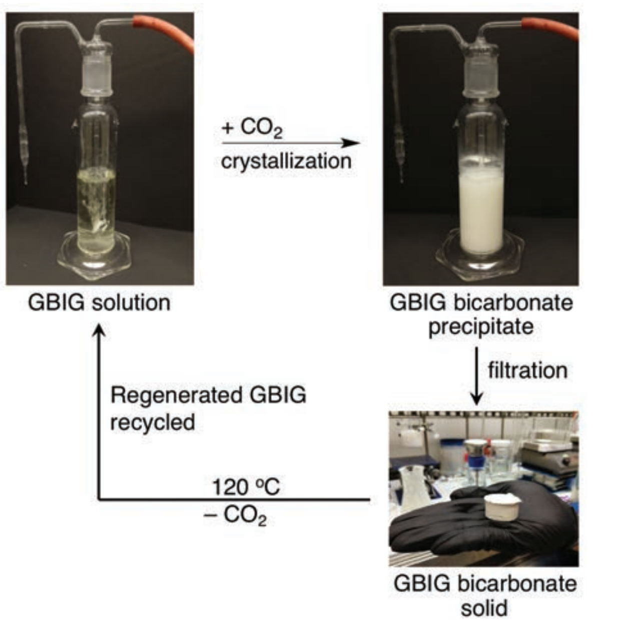

Figure 2. CO_2 separation via GBIG bicarbonate crystallization [7]. A flue gas simulant (12.8% CO_2, EPA standard) was bubbled through an aqueous GBIG solution (a), leading to crystallization of GBIG bicarbonate (b). The solid was collected by filtration and heated at 120°C to release the CO_2 and regenerate the GBIG sorbent (c). The filtrate containing the residual GBIG and regenerated GBIG solid was recycled (d) [7].

Although GBIG efficiently captures CO_2 from flue gas, it is inadequate for DAC. In this effort, exposure of an aqueous GBIG solution to air simply led to crystallization of the hydrated GBIG. Nonetheless, by taking advantage of the modular nature of BIGs and their straightforward syntheses, an analogous compound, 2,6-pyridine-bis(iminoguanidine) (PyBIG), was formed that proved to be very effective for DAC [9]. An aqueous solution of PyBIG open to air reacted with atmospheric CO_2 and crystallized as a hydrated carbonate salt (Figure 3). The very low aqueous solubility of the PyBIG carbonate salt, on par with limestone, drove the crystallization equilibrium despite the very low concentration of CO_2 in the air. A structural factor contributing to the low solubility of the PyBIG carbonate salt was the strong hydrogen bonding of the carbonate anions by the guanidinium groups and the water molecules included in the crystals. This was found through single-crystal neutron diffraction combined with electron density measurements from high-resolution x-ray diffraction [10]. Mild heating of the carbonate crystals at 80°C–120°C released the CO_2 and regenerated PyBIG quantitatively, thereby closing the CO_2-separation cycle.

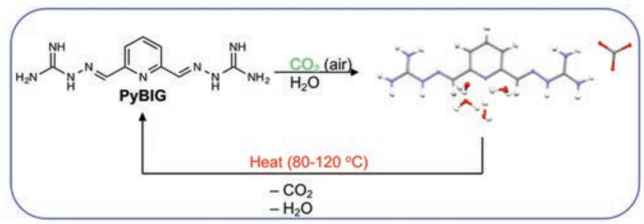

Figure 3. DAC with PyBIG via crystallization of a hydrated carbonate salt. The crystal structure of the PyBIG carbonate salt, as determined by single-crystal neutron diffraction, is shown at right [9].

The efficiency of DAC with BIGs can be tuned via crystal engineering [11]. Relatively minor modifications in the molecular structure of GBIG, such as substituting one or two hydrogen atoms with methyl groups, led to dramatic differences in (1) the crystal structures of the resulting methylglyoxal (MGBIG) and diacetyl (DABIG) analogs and (2) their aqueous solubilities and DAC performance [12]. Notably, the low solubility of the carbonate salts of MGBIG and DABIG compared with the neutral BIGs provides the thermodynamic driving force for the corresponding DAC reactions, as shown in Figure 4.

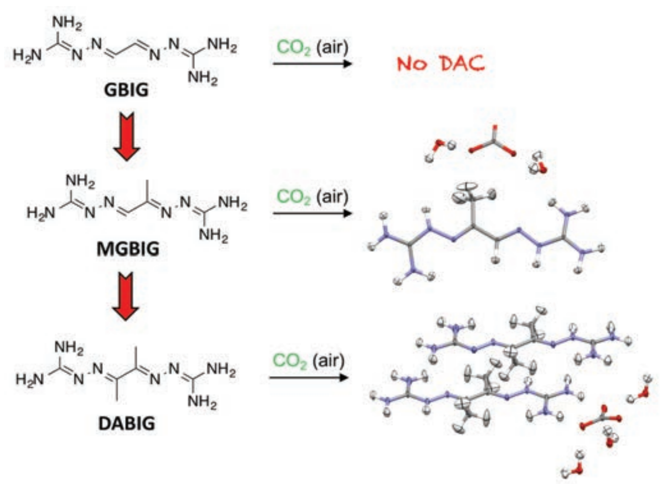

Figure 4. Dialing in DAC by crystal engineering of BIGs [11]. An aqueous solution of GBIG left open to air led to crystallization of the free compound, whereas the corresponding solutions of the methylated analogs MGBIG and DABIG led to DAC [12].

DAC with amino acids–BIG hybrid systems. Another strategy to boost the DAC performance of BIGs is to combine them with aqueous amino acids [5] or peptides [6], significantly enhancing CO_2 capacity and absorption rates. In these hybrid systems, simple amino acids like glycine or sarcosine, or small oligopeptides like glycylglycine, react quickly with atmospheric CO_2 and convert it into bicarbonate anions. A household air humidifier (Figure 5A) was used to facilitate the mass transfer of CO_2 from air into the aqueous amino acid or peptide solutions. The humidifier consisted of a reservoir containing the aqueous solvent, a rotating wick that spread the solution into a thin film to enhance its contact area with the air, and a fan that blew air over the wick. Although this configuration was not optimized for DAC, it served as a simple, economical setup for the initial proof-of-concept experiments. BIG solids were then added to the loaded amino acid solution, leading to crystallization of BIG carbonate salts and regeneration of the amino acid, which was recycled. Finally, mild heating of the BIG (bi)carbonate crystals released the CO_2 and regenerated the BIG solid, which was also recycled. Heating methods that avoid the use of energy sources that emit CO_2 are an important consideration in DAC process design: regeneration of PyBIG with concentrated solar power as a renewable source of energy was demonstrated using a solar oven (Figure 5B) [5].

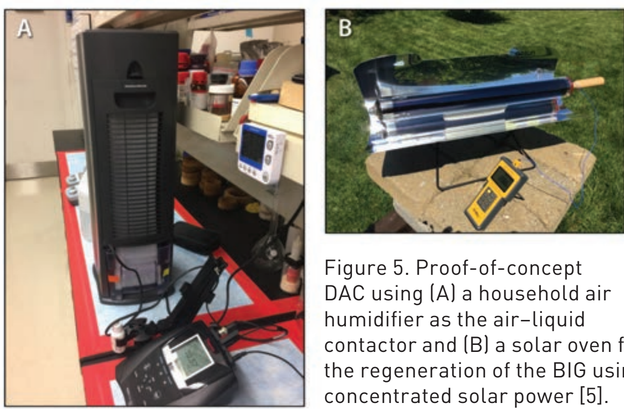

Figure 5. Proof-of-concept DAC using (A) a household air humidifier as the air–liquid contactor and (B) a solar oven for the regeneration of the BIG using concentrated solar power [5].

From basic science to DAC technology development and commercialization. Although the initial fundamental studies provided information about the factors controlling DAC efficiency with BIG–amino acid systems, more R&D efforts are needed to transform this basic discovery into an energy-efficient, cost-effective DAC process that can be deployed at the much larger scale necessary to mitigate climate change. Specifically, the chemistry must be optimized to maximize the CO_2 cyclic capacity and absorption rate, as well as sorbent lifetime. The CO_2 uptake appears to be limited by mass transfer from air into the aqueous amino acid solution, thereby requiring the design of an efficient air–liquid contactor. Next, a crystallizer and a solid–liquid separator must be developed to handle large volumes of slurries/solids and to operate under continuous crystallization conditions. CO_2 release from the BIG carbonate crystals also must be optimized to minimize the time, temperature, and energy required and to maximize heat flow and integration. The use of renewable or waste-heat energy sources must be exploited as much as possible to increase sustainability of the DAC process. Finally, the entire system (Figure 6) must be run continuously for thousands of cycles to optimize all parameters and to collect the necessary data for a realistic technoeconomic

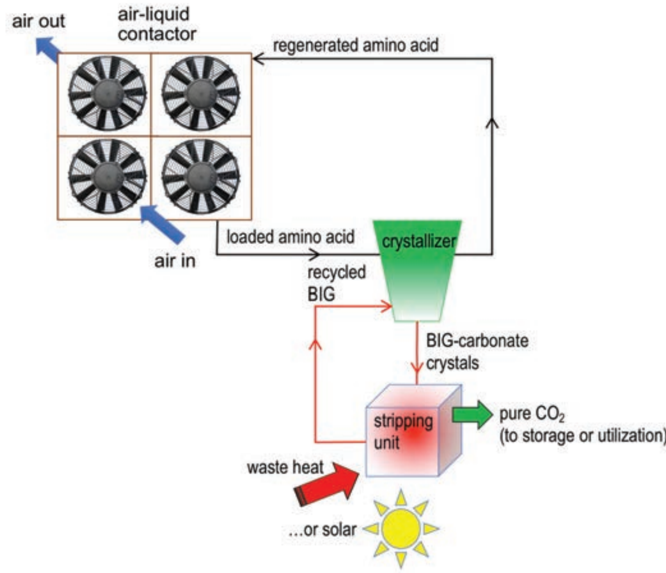

Figure 6. DAC process flow diagram in development at ORNL based on an amino acid–BIG sorbent system [8].

analysis. These applied research activities are currently being pursued at ORNL, with the ultimate goal of developing and maturing a bench-scale DAC technology that can be scaled up and commercialized.

Moving forward, a critical step is to identify industrial partners interested in BIG DAC commercialization. ReactWell, a company based in New Orleans, Louisiana, has partnered with ORNL to develop an integrated process for DAC and electrochemical conversion of CO_2 to ethanol for use in fuels or hand sanitizers. Another company, Holocene Climate Corporation, performed a preliminary technoeconomic analysis that estimated that the cost of DAC by BIG crystallization is competitive with existing DAC technologies from Carbon Engineering and Climeworks. Holocene intends to license and scale up the ORNL technology to eventually remove billions of tons of CO_2 per year from the atmosphere for permanent geologic storage.

IMPACT

ORNL, ReactWell, and Holocene won an R&D100 award in 2021 for the DAC technology discussed in this article. Further development, optimization, and scale-up in collaboration with private partners will result in a commercial DAC technology being deployed worldwide to permanently remove billions of tons of CO_2 from the atmosphere to mitigate climate change.

COLLABORATE WITH ME

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Decarbonization of Concrete

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INTRODUCTION

The manufacture of building materials is responsible for 10% of all anthropogenic CO_2 emissions and for 26% of all emissions attributed to the buildings sector [1]. The building material that contributes most to the industry's carbon emissions is Portland cement, the binder used to produce concrete. The manufacture of Portland cement is energy- and carbon-intensive because it involves high-temperature heat treatment of a mixture of raw materials that includes limestone, which decomposes and releases carbonic gas to the atmosphere during the kilning stage. For each ton of cement produced, it is estimated that an average of 0.9 tons of CO_2 are emitted [2]. Even though cement's carbon footprint is small compared with many other materials [3], the cement industry is responsible for 8% of the global anthropogenic emissions of CO_2 [4] because of its scale of use.

Portland cement–based concrete is the material that is manufactured by humans in the largest amount, exceeding all other materials combined. It is the main material used in urbanization and infrastructure of cities because it is cheap and versatile and can be prepared and applied by unskilled laborers in the construction of the simplest or most complex structures. Annual global production of concrete is estimated to be ~10 billion cubic meters (13 billion cubic yards) [5], corresponding to 4 metric tons per capita per year considering the world's population. In the United States, ~250 million cubic meters (330 million cubic yards) of concrete were placed in 2012 [4]. Each ton of concrete contains an average of 0.10 tons of Portland cement [5]. Cement is also used in a multitude of other building materials such as pipes, blocks, pavers, tiles, and mortars. This large-scale use is the main reason for the construction sector's high CO_2 emissions. However, given the advantages offered by Portland cement–based concrete (i.e., its simplicity of use and worldwide availability) and the pressures to address the housing deficit forecasted for the coming decades, it is unlikely to be replaced by any other technology soon.

Concrete is a mixture of Portland cement, water, sand, stone, and small amounts of chemical admixtures. Most concrete formulations contain supplementary cementitious materials (SCMs) that partially replace Portland cement to reduce cost, to achieve desired concrete properties, and more recently, to reduce the carbon footprint of cement and/or concrete. SCMs react with the hydration products of cement to form strength-bearing phases to enhance the performance of the final product. They include ground limestone rock; fly ash, a residue from coal combustion in power plants; blast furnace slag, a byproduct from the purification of iron ore; volcanic ashes; and calcined clays.

In 2015, the United Nations Environmental Programme Sustainable Buildings and Climate Initiative assembled a group of academic and industrial experts from several countries to evaluate low-carbon technologies for cement-based materials. The group concluded that two main measures could substantially reduce the carbon footprint of the industry in the near term [6]: increasing the use of SCMs to replace cement, and improving the efficiency of Portland cement use in construction to decrease the amount of cement needed for the same product functionality. This second measure includes the use of efficient concrete designs and specification of higher-grade strength concrete when the total amount of materials consumption can be reduced. Other emerging technologies to reduce carbon emissions by the buildings sector—such as alternative chemistry binders and carbon capture use and/or storage—are still in early development and can help reduce carbon at scale only over the long term (i.e., >20 years from now) [6].

The ORNL Building Envelope Materials Research (BEMR) Group is developing technologies to reduce the use of cement in the manufacture of concrete while minimizing the industry's overall generation of waste. One of these projects, funded by the US Department of Energy Building Technologies Office, aims to deploy a concrete design technology that reduces the consumption of cement by 35 to 70% by maximizing the packing density of the granular system, hence reducing porosity, water consumption, and embodied carbon without penalties to concrete performance. A seed money project will investigate whether Portland cement can be fully replaced by a binder based on coal ashes harvested from deposit ponds. A technical collaboration is in process to scale up the partial substitution of Portland cement in concrete with low-grade calcined kaolinitic clays. Other exciting ideas with great potential to decarbonize building materials in the long term are also being explored, including replacement of cement with earth-based and biopolymeric binders. All projects involve industrial partners to accelerate the development and deployment of solutions, including a professional association, an energy company, and a global supplier of minerals. Some of these efforts are described herein.

EFFICIENT CONCRETE DESIGN

Several factors are considered when designing concrete formulations that include the properties and characteristics of the raw materials (e.g., chemical and mineralogical compositions, physical properties) and of the concrete (e.g., flowability, setting time, strength, durability). If concrete constructions are effectively designed, built, and maintained, they can last several decades or even hundreds of years.

We have a great opportunity to increase the efficiency of cement use in concrete through better mixture designs to reduce CO_2 emissions [5]. The efficiency of Portland cement in concrete can be expressed as binder intensity (BI), which represents the amount of cement in a unit volume of concrete necessary to deliver a unit of strength. Figure 1 shows a comparison between conventional concrete mixes (gray) and optimized concrete formulations (all other colors) and as published in [7]. The BIs for most of the conventional designs range from 5 to 15 kg/m3.MPa. With the efficient concrete design approach, BIs as low as 2 kg/m3.MPa can be obtained, even for high-strength concrete.

The approach involves using (1) an optimized particle size distribution to maximize packing density, (2) a filler with particle sizes similar to those of the cement, (3) an ultrafine filler to occupy the spaces between the cement and the filler particles, and (4) a dispersant dosed in enough content to ensure deagglomeration of the fine and ultrafine fillers [8]. This approach has the potential to reduce cement consumption by at least 35%, and it could reduce water content by at least 10%–15% compared with conventionally designed concrete. Simultaneously reducing cement and water content maintains and improves concrete performance parameters. Including fine and ultrafine particles—or fillers such as ground limestone and quartz—further reduces the porosity of the mix, resulting in a denser microstructure that is less permeable to the transport mechanisms associated with concrete deterioration. In addition, this approach results in less cracking from shrinkage

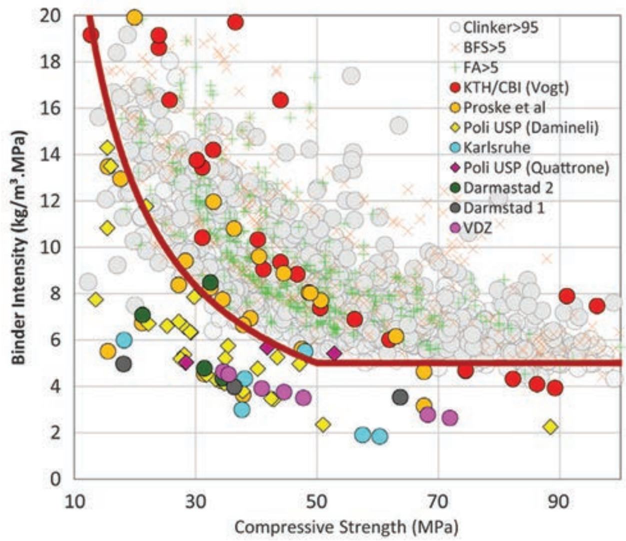

Figure 1. Data related to BI of concrete from 156 randomly selected articles published between 1988 and 2009 from 29 countries [7]. Gray indicates conventionally designed concrete mixes, and all other colors represent efficient concrete designs. The red line identifies the limit for conventional concretes. (Credit: John et al.)

and thermal gradients because the system's porosity and Portland cement content are lower than that of traditional concrete.

ORNL's BEMR Group is working with precast concrete producers to deploy this technology. The following benefits are expected:

- Multifold reduction of BI, with associated reduction in CO_2 intensity
- Superior concrete mechanical performance, with the ability to cast concrete elements in smaller dimensions that use less concrete
- Lower shrinkage and lower heat of hydration, resulting in less cracking and higher durability
- Lower porosity and permeability, leading to superior durability
- Cost neutrality or cost reduction compared with current concrete production practices
- Minimal adjustments to current concrete production practices
- Minimal capital investment by concrete producers

Full deployment of this technology at partner concrete plants is expected within the next 2 years, with rollout to the broader concrete industry expected thereafter. If the technology is implemented in ~30% of US concrete designs, industry CO_2 emissions would be reduced by 11 million tons annually, assuming that production of 1 m3 of concrete results in the emission of 240 kg–320 kg CO_2eq [4].

HARVESTED COAL ASH BINDER

Fly ash, a by-product from coal burned in power plants, has been used for several decades to replace part of the Portland cement in cement-based materials such as concrete because of its lower cost and superior durability. Fly ash also helps reduce concrete's embodied carbon, although this was not a driver until recently. However, in the past 10–15 years, the quality and availability of fly ash have decreased in the United States as a result of (1) increasing use of technologies that remove greenhouse gases and other pollutants from flue gas and (2) the decommissioning of almost 300 power plants [9]. The decreased availability of standard-compliant quality fly ash and the consequent price increase are putting pressure on concrete producers, the main users of fly ash, to implement beneficiation techniques or to find materials other than fly ash.

These issues have led to a growing interest in using fly ash that has been disposed of in ponds and landfills. It is estimated that US reserves of coal combustion residues are nearing 1 billion tons [10] as a result of decades of disposal. Diaz-Loya et al. [11] dried and classified fly ashes ponded 40–50 years ago, demonstrating that they were sufficient to provide performance similar to newly generated ashes collected from silos at the same power plant. No important chemical or mineralogical differences were detected between the two sources. After beneficiation, the harvested ash fulfilled the requirements of ASTM C618-19 [12], which is the standard for compositional and physical characteristics of fly ashes used in concrete. Conversely, Wirth et al. [13] detected the presence of hydrated phases and morphological differences between ponded and fresh ashes, indicating that significant changes might occur during weathering. Calcium content in ash composition is an indication of its reactivity in water. ASTM C618 Type C (high calcium) fly ashes have hydraulic cementing properties, whereas Type F (low calcium) ashes, the most common type, is mostly inert when in contact with water. Harvested coal ash might also require treatment to remove organic matter and other contaminants [13]. Coal combustion residues (CCRs) other than fly ash are discarded in ponds and landfills. These CCRs include bottom ash, boiler slag, fluidized bed combustion ash, and other fine particles [14,15]; contamination of fly ashes with these CCRs is expected. Fly ashes must comply with the ASTM C618-19 requirements for use in concrete. Excessive content of contaminants such as sulfur and unburnt coal particles renders the material unusable.

Coal ash ponds pose threats to human health and the environment. CCRs contain chemical elements of environmental concern, such as antimony, arsenic, barium, beryllium, cadmium, chromium, lead, mercury, nickel, selenium, silver, and thallium [15]. Because CCRs deposited in ponds are in continuous contact with water, these elements leach, and in unlined containments, they contaminate the groundwater over time [16,17]. Harkness et al. [18] analyzed samples from 22 sites in 5 states in the southeastern United States (i.e., Tennessee, Kentucky, Georgia, Virginia, and North Carolina) and found strong evidence of surface or subsurface leaking of coal ash ponds and, in some cases, contamination of nearby water sources. In 2014, Goemann [17] reported the existence of ~630 coal ash ponds in use at 495 coal-fired power plants throughout the United States, and 207 ponds in 37 states were found to have contaminated water or air above the limits established by federal health standards. In addition, structural pond failures have led to more than 1.26 billion gallons of residues flooding into waterways and communities near coal-fired power plants between 2003 and 2013, including the coal fly ash spill in 2008 in Kingston, Tennessee [19].

Coal ash harvested from ponds and landfills can be a valuable raw material not only for use in conventional concrete but also, and more interestingly, for use in alkali-activated binders (AABs), which may have much lower embodied carbon than cement-based materials. AABs are formed by the alkali activation of alumino-silicate sources (or precursors), from naturally occurring or synthetic materials or industrial waste [20]. The first AABs were developed in the 1950s in Ukraine using blast furnace slag [6]. Since then, other precursors have been investigated and used in several applications, including fly ash and metakaolin [21]. Long-term exposure of AABs, both in service and in laboratories, has shown that these materials are robust and durable and have the potential to replace cement-based materials for both structural and nonstructural applications [22]. The carbon emissions of AABs can be lower than those from Portland cement–based systems, depending mostly on the type of alkali activator used [23]. For example, sodium silicate, the most used alkali activator in AABs, is estimated to be responsible for about half of the embodied carbon of the binder. Alternately, sodium hydroxide and sodium carbonate have a much lower global warming potential [24].

Harvested ashes can be more suitable to use in AABs than in Portland cement systems because AABs can be produced from bottom ash and boiler slag [25], which are contaminants present in the pond. In addition, fly ash–based AABs immobilize several heavy metals, including zinc, copper, chromium (III), cadmium, and lead, demonstrating that the oxides of these metals can be distributed uniformly within the matrix [26]. However, arsenic and chromium (VI) appear to be weakly bonded [27], so leaching tests must be performed to ensure that they are not removed from the AAB after hardening.

The use of harvested coal ashes to produce AABs will help overcome one of the most important challenges for widespread use of the technology: the local availability of precursors. Another major obstacle to scaling up AAB technology involves the alkali activator. Even though sodium silicate is the most common activator used in AABs, it is the least attractive option in terms of cost, availability, and embodied carbon. Other options for alkali activators exist: biomass ashes, red mud, waste glass, diatomaceous earth, silica fume, and other alkaline waste sources might be appropriate alkali activators for AABs with low embodied carbon [28]. Using harvested ashes to produce AABs could reduce the volume of impoundments, decrease the leaching of heavy metals to waterways, and reduce the risk of the containments' structural collapse.

The BEMR Group collaborates with a US energy company to advance the research and overcome obstacles for wider adoption of low-carbon binders while addressing human health and environmental risks of fly ash ponds. Work is underway to evaluate the suitability of minimally processed harvested coal ashes from ponds and/or landfills to produce AABs and to identify possible sources of alkali activators, preferably from waste streams. Leaching tests will be performed on heavy metals from the binders to investigate whether toxic elements can escape the AABs.

LIMESTONE/CALCINED-CLAY CEMENTS

Calcined clay represents the greatest opportunity to extend the use of SCMs because of its worldwide availability. Ordinary clays containing 40%–60% kaolinite develop strong chemical (i.e., pozzolanic) activity if calcined to temperatures not higher than 850°C. Calcined smectite, bentonite, and montmorillonite clays can also develop pozzolanic reactivity [29]. During thermal treatment of clays, there is no CO_2 release, and the calcination temperature is, importantly, lower than that of Portland cement kilning, making calcined clay a lower embodied carbon substitute to cement. When used in combination with limestone, cement substitute can be as high as 50% because calcined clay and limestone's calcium carbonate react to form strength-bearing phases [30].

The availability of clay for use as a cement substitute is considered unlimited given the size and location of reserves. Existing quarrying operations for other applications represent an enormous potential to increase the global supply in some countries [6]. Clay-rich dredged sediments from ports, harbors, and waterways are another possible local source [31,32].

Even though reserves abound, the supply of calcined clays is not well established in most parts of the world. The BEMR Group is working with a major global mineral supplier to identify combinations of calcined clays and other ingredients to provide optimum performance to concrete mixes, aiming to accelerate the deployment of this technology in the United States.

CONCLUSIONS

The most recent report released by the Intergovernmental Panel on Climate Change on April 4, 2022 [33], states that immediate and deep emissions reductions across all sectors must be pursued to limit global warming to 1.5°C. According to the report, deployment of technologies with high readiness levels should be the industry's immediate focus. The authors also emphasized that more efficient use of materials, higher reuse and recycling of products, and minimization of waste will be required to reduce emissions.

Substantial decarbonization of the construction sector is possible in the short term to midterm by reducing the use of Portland cement in the manufacture of building materials, achievable by increased efficiency in design and construction and an increase in the use of supplementary cementitious materials. To this end, ORNL's BEMR Group is collaborating with scientists from other ORNL groups, external research organizations, and industry to research, develop, deploy, and demonstrate technologies that, when adopted at scale, are expected to reduce the CO_2 emissions of the Portland cement industry by at least half of the target reductions [34].

IMPACT

If adopted at scale, the technologies described herein could contribute to the reduction of at least 50% of the target emissions by the cement industry. In addition, broader use of harvested coal ashes in building materials will reduce the human and environmental risks imposed by long-term storage ponds. The following major achievements are possible: decreased embodied carbon of Portland cement–based materials, identification of a safe repository for coal ashes from storage ponds, and coupling of large amounts of unused ash and calcinable clays with vast amounts of concrete and other Portland cement–based materials to be used by the construction industry.

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Optimizing Plant Traits for Bioenergy and Soil Carbon Storage

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INTRODUCTION

One of the most promising natural methods for removing carbon from the atmosphere involves stabilizing organic carbon in soil, which has a large and underexplored storage capacity. Carbon storage in working agricultural landscapes is seen as particularly promising, with an estimated sequestration potential of up to 0.25 Gt C/year in the United States and 3 Gt C/year globally [1]. Public perception of natural CO_2 removal solutions is positive, and implementation using bioenergy and agricultural crops can be conducted using existing technology.

BACKGROUND

Plant traits can be optimized to promote storage of soil carbon and thereby contribute to CO_2 removal. Specific plant traits are controlled by plant genetics, which have previously been identified through analyses at ORNL of the bioenergy crop *Populus trichocarpa* [2]. Essentially, ORNL's database contains most of the possible variations of *Populus's* entire genome. In this project, genomic information is being used to target specific plant traits that could influence soil carbon. This massive genomic database resource is not available for most plants or to most researchers. Consequently, this project has the potential to innovate the design of bioenergy cropping systems. The challenge remaining for this project is that measurements of aboveground plant traits are common, while carbon storage is largely controlled by belowground plant traits (e.g., root biomass, root tissue chemistry, and microbial activity). Belowground traits are not commonly measured because of the lack of available nondestructive methods for detecting root biomass in the subsurface. More research is needed to understand how root tissue chemistry and microbial activity influence the persistence of dead roots within soils and the transformations

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of root tissues into long-lived soil organic matter. Therefore, using genomic information is a promising method to predict particular plant traits, but linkages between genomic information and actual belowground traits remain to be directly measured.

In this project, we hypothesize that some plant traits can reduce the ability of microbes to decompose root tissues and thereby promote the accumulation of the materials in soil organic carbon. Specifically, plants pump or leak chemicals referred to as metabolites through their roots and into the soil. These metabolites can inhibit the ability of soil microbes to perform specific tasks [3], such as the ability to decompose organic materials such as decaying roots. The chemistry of the roots themselves can also influence the rate and extent of microbial decomposition when roots die. For example, lignin is a class of plant chemical compounds that provides structural rigidity to plant tissues. Higher amounts of lignin or more resistant forms of lignin can reduce the ability of soil microbes to decompose plant materials because lignin is not as easily decomposed as other plant materials, such as cellulose, under most conditions. These specific plant characteristics are being identified from existing genomic analyses in *Populus* [4], and the effects of those plant traits on soil carbon will be determined in this project.

RESULTS

Plant traits. The plant metabolites ferulic acid and para-coumaric acid are released by plant roots into soils. These two metabolites can independently inhibit decomposition of plant tissues by soil microbes. The ratio of two different monomers of the large and complex lignin molecule—syringil to guaiacyl—can provide an indication of the degradability of the lignin in root tissues. A high syringil-to-guaiacyl ratio in plant tissues is thought to inhibit microbial decomposition and promote preservation of plant tissues within soil organic carbon.

Soils have been collected from six *Populus* genotypes for each of these three plant traits, where three genotypes (with replication) have been targeted to maximize the trait and three genotypes (with replication) have been chosen to minimize the trait. Comparison of soil carbon between these trait extremes will enable the determination of the effect of that particular plant trait on soil carbon. Root samples from each tree have also been collected to analyze for lignin content, carbon and nitrogen, and other nutrients (Figure 1). The soils were characterized according to standard methods for pH, moisture content, texture, carbon and nitrogen content, and microbial biomass. Each of these properties could provide a complementary or confounding influence over carbon storage.

Soil carbon. Previous studies tended to focus only on the total amount of carbon. Here, soils are physically fractionated into particulate and mineral aggregate fractions, where particulate organic carbon fractions mostly reflect preservation of plant tissue residue materials and mineral-associated fractions reflect microbial decomposition of plant materials and subsequent association of the partially decomposed product with soil minerals [5]. Therefore, the fractionation method will enable key understanding about how specific plant traits influence the characteristics of soil organic carbon. More importantly, the ability of soils to incorporate new carbon, and its longevity, depends on its form: soils tend to have a high capacity for particulate organic carbon, which can remain in soils for years to decades [6]. And while soils have a finite capacity for mineral-associated carbon, this form of carbon might be preserved for decades to centuries because association involves direct chemical bonding to soil minerals [6]. To gain further understanding of the mechanisms contributing to the form and preservation of soil carbon, the particulate and mineral-associated fractions will also be analyzed by Fourier-transformed ion cyclotron resonance mass spectroscopy (FT-ICR-MS), which is available through user proposals to the DOE Environmental Molecular Sciences Laboratory. FT-ICR-MS is a high-throughput method that can provide estimates of the oxidative status of soil organic carbon and the extent of lignin, cellulose, aliphatic, and aromatic compounds remaining in soil organic carbon [7]. Differences might be observed in the chemistry of particulate versus mineral-associated organic carbon, where particulate carbon might retain more characteristics of the plant tissues compared with the composition of mineral-associated carbon. Determination of the oxidative status can further indicate the extent of microbial decomposition, where greater oxidative status implies more decomposition.

Figure 1. Roots can incorporate soil organic material and promote carbon storage. (Credit: Melanie Mayes)

CONCLUSIONS

This project serves as proof of principle for the role of plant traits in bioenergy crops to specifically affect the rates and mechanisms of the storage of soil organic carbon. Enhancing soil carbon storage is one of the simplest and most economical methods to remove carbon from the atmosphere, particularly if associated with biofuel production. We aim to demonstrate how genomic phenotyping, an area in which ORNL is already a global leader, can be harnessed to enable bioenergy cropping that measurably increases soil organic carbon and enables net-negative emissions. The project also provides foundational knowledge on relationships between plant traits and mechanisms of soil organic carbon accumulation such as mineral associations and stabilization of plant tissue residues.

IMPACT

The effects of increased soil carbon from trait optimization in bioenergy cropping can be modeled to determine its regional, national, and global potential, and plant traits in both *Populus* and other biofuels can be selected that will alter soil carbon storage in bioenergy and other cropping systems.

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Analyzing the Best Uses of Biomass for Energy-Sector Decarbonization via an Integrated Carbon Management Approach

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INTRODUCTION

Domestically grown, sustainable biomass is an increasingly important resource for our nation's decarbonization goals. Current bioenergy use in the United States is ~4 quadrillion (10^{15}) BTUs (quads), which could increase to 15 quads if we take full advantage of the approximate billion-ton potential of biomass. The question is, where can those resources be best allocated, given that the decarbonization needs of the various energy sectors exceed available biomass? To understand the best uses of biomass, we must perform new types of analyses across different routes and pathways, recognizing the competing end-use energy sectors as we move toward our 2050 decarbonization goals.

BACKGROUND

Using fossil fuels for energy production releases carbon that has been in the ground for millions of years, increasing carbon in the atmosphere and contributing to the climate crisis. ORNL led the effort to develop the *Billion-Ton Report* for the US Department of Energy's (DOE's) Bioenergy Technologies Office to understand the potential of biomass resources that can be allocated to energy production in the United States [1]. Biomass for energy production can be grouped into numerous categories: conventional agricultural land resources (grains and oilseeds); herbaceous energy crops (switchgrass, miscanthus); agricultural residues (corn stover, wheat straw); woody biomass and energy crops (forestland resources or woody crops); algae; and wastes (black liquor, mill wastes). Each of these biomass resources has a regional (i.e., spatial) aspect that impacts the cost of energy production and transportation, as well as the total carbon emissions.

Biomass is sustainable in that plants draw in carbon during the growing process and then release the carbon during energy production and usage, but the net effect from the biomass itself is fairly carbon-neutral, as illustrated in Figure 1.

The processes around growing and harvesting biomass all require energy, including fertilizer produced using fossil-based natural gas and harvesting equipment powered by petroleum-based diesel fuel, so each of those steps result in the emission of carbon into the atmosphere. Transportation of biomass by truck, rail, or barge will result in additional emissions of carbon due to the petroleum-based fuels powering the fleet. Production of energy from biomass often requires energy for the conversion process, and that energy might come from fossil fuels. All these processes result in emissions that must be included in the carbon accounting. If any of these processes are fueled by sustainable energy (e.g., biodiesel, renewable natural gas, green ammonia fertilizer), those emissions can be considered "clean" in that they do not increase the carbon in the atmosphere.

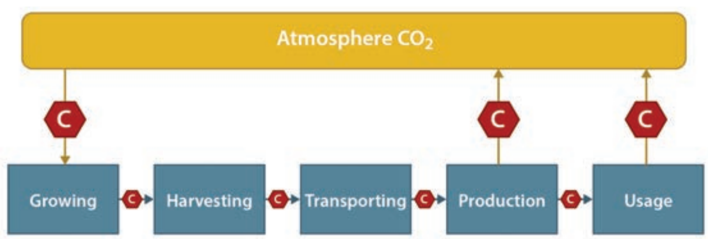

Figure 1. Biomass carbon cycle. (Credit: Ingrid Busch, ORNL)

Certain carbon benefits can also be taken into account. Some types of biomass transfer carbon to the soil as part of the growing process. The extent of this soil sequestration depends on the type of biomass and the type of land use (e.g., crop, pasture). Additionally, carbon can be captured during the energy production process and then sequestered in geological formations. This results in the more complete carbon accounting cycle shown in Figure 2.

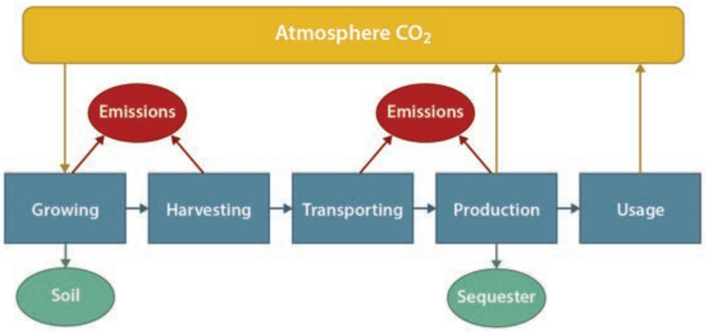

Figure 2. Complete carbon cycle. (Credit: Ingrid Busch, ORNL)

METHODOLOGY

To meet the overarching goal of decarbonizing all US energy sectors, we must first understand and then strategically apply limited resources to have the maximum impact on avoiding and eliminating carbon emissions. This includes understanding the carbon avoidance cost of the potential pathways (i.e., the cost of replacing fossil products with biomass-derived alternatives relative to the amount of emission avoided).

Potential areas for siting US bioenergy facilities were generated using the Oak Ridge Siting Analysis for Power Generation Expansion (OR-SAGE) model [2]. Exclusion criteria given to OR-SAGE included population centers, wetlands and open water, protected lands, landslide hazards, and 100-year floodplains. Requirements for suitable sites also included the availability of cooling water with sufficient flow within 20 mi. These suitability criteria resulted in the areas shown in Figure 3.

When carbon capture and sequestration (CCS) at the production facility is included in the analysis, the sites that can accomplish this are required to sit directly on a suitable geologic formation for direct sequestration. Future work will include the modeling of the transportation of the CO_2 (by fleet or by pipeline) to locations suitable for sequestration.

Figure 3. Suitable areas for bioenergy facilities. (Credit: Ingrid Busch, ORNL)

This analysis uses the ORNL-developed BILT (Biofuel Infrastructure, Logistics and Transportation) model for supply chain analysis (Figure 4). This accounting model tracks the entire biomass-to-end-use supply chain, which includes biomass production, transportation, and processing, for potential feedstocks, pathways, and end uses. This model relies on critical inputs from peer-reviewed technoeconomic analysis (TEA) and life cycle analysis (LCA) for key economic and carbon cycle data of these routes with different pathways. For this analysis,

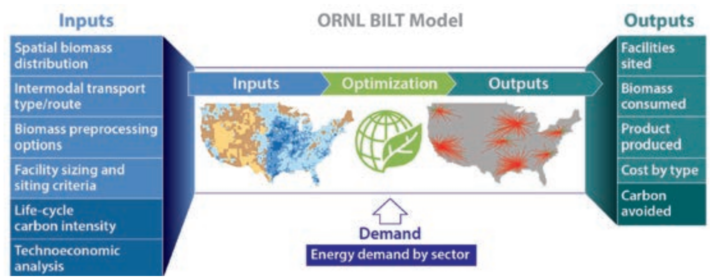

Figure 4. BILT model process. (Credit: Brett Hopwood, ORNL)

it is important to have county-level spatial resolution across all ~3,100 counties in the United States, as well as LCA and TEA inputs to understand how location can affect both carbon intensity and cost. The analysis is done for both the near term (using feedstocks that are currently available) and long term (circa 2040, when the market for herbaceous crops is expected to be available). Figure 5 shows an example of the US distribution by county of herbaceous energy crops including miscanthus,

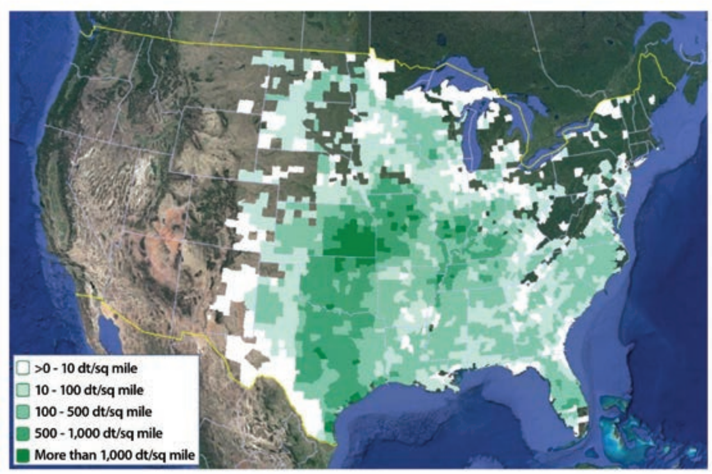

Figure 5. County-level resolution on biomass allocation for herbaceous energy crops with values shown in dry ton per square mile. (Credit: Ingrid Busch, ORNL)

switchgrass, biomass sorghum, and energy cane using the 2040 Billion-Ton Study Spatial Distribution at a price of $60/dry ton [1].

Figure 6 illustrates the amount of biomass available as the price offered per ton increases.

RESULTS

This work describes a new, integrated biomass use analysis approach to selecting biomass best uses (Figure 7) developed

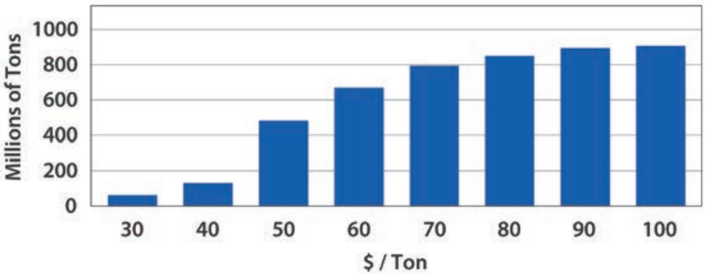

Figure 6. Biomass availability from the 2040 Billion-Ton Study. (Credit: Langholtz et al.)

at ORNL and how it can be applied to three competing routes: (1) use biomass directly for biopower to serve the electrical sector; (2) convert biomass into renewable natural gas (i.e., methane) to serve the industrial sector; and (3) convert biomass into different biofuels for the competing aviation, ground transportation, and maritime transportation sectors. All three routes can be considered with or without carbon sequestration at the conversion facility. The biogas route leverages the nation's natural gas pipeline network to transport natural gas from biomass, coupled with CCS to remove CO_2 from the air.

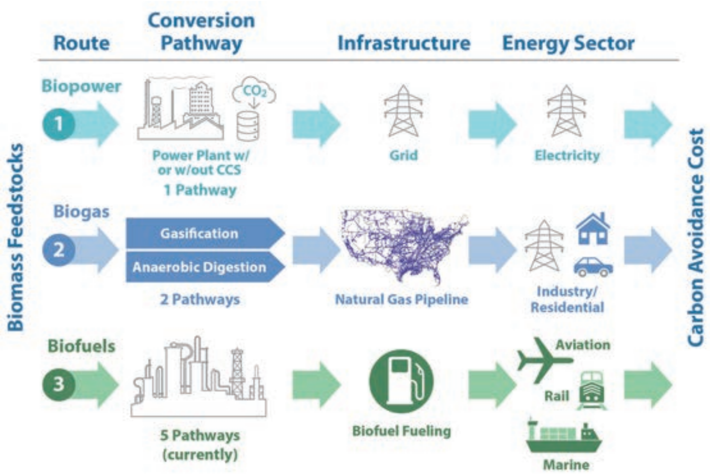

Figure 7. Best uses of biomass for decarbonization with competing pathways. (Credit: Brett Hopwood, ORNL)

CONCLUSIONS

While this research is ongoing, this methodology allows analysts to compare potential uses for the limited biomass that is expected to be available and provides insights into how allocations of the biomass to the pathways can best be used for the nation's decarbonization efforts.

IMPACT

This approach will help decision-makers select the most impactful and cost-effective feedstock allocations. In addition, this analysis will help provide additional understanding regarding investment needed, elucidate the region-specific benefits and challenges for a particular product, and help identify opportunities for biomass resources to provide economic, environmental, and social benefits.

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Unlocking US Biomass Potential

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INTRODUCTION

Nations around the world are seeking ways to support economic development while mitigating the potential negative impacts of climate change. Under the Paris Climate Accord, each nation needs to implement policies to achieve net-zero emissions by 2050. Burning gasoline and other fossil fuels emits CO_2 to the atmosphere, a primary cause of climate change. Thus, governments aim to both reduce fossil fuel use and increase carbon sequestration.

Biomass is one tool for achieving this goal. When plants grow, they remove CO_2 from the air and convert it to biomass. With variable levels of processing, biomass can be used to replace a wide variety of products that currently require large amounts of fossil materials and energy. For example, biomass can be used to generate power and electricity and as an alternative to plastic, steel, and concrete. Biomass can be converted to biofuels or other forms of bioenergy to replace fossil gasoline and diesel in vehicles or coal and natural gas in power plants. When fossil inputs are avoided, they remain sequestered in the ground, whereas biomass forms one part of a constant, natural cycling of carbon. Thus, large net reductions of carbon and other climate-forcing emissions can be avoided with proper production and use of biomass.

Biomass can even provide net-negative emissions when combined with bioenergy with carbon capture and storage (BECCS). BECCS is one of the key technologies identified in the new report from the Intergovernmental Panel on Climate Change (IPCC Sixth Assessment Report) on actions necessary to achieve climate change mitigation targets because BECCS takes biomass carbon captured from the atmosphere by plants and sequesters it via geological storage. Yet, questions persist regarding the availability of sustainable biomass required to achieve the IPCC targets.

BACKGROUND

The ORNL-led US Department of Energy 2016 "Billion Ton Study" (BT16)[1] has been the gold-standard estimate of sustainable biomass production potential in the United States [1]. The potential for biomass supplies based on documented technoeconomic assessments is estimated by resource type and amounts to more than 1,000 million Mg (metric tons) per year in a base case for near-term supply potentials. More recently, ORNL researchers have collaborated with the Energy Futures Initiative (EFI)—a nonprofit research organization led by former Secretary of Energy Ernie Moniz dedicated to harnessing the power of technology and policy innovation to accelerate the clean energy transition—to update and expand the BT16 estimate of sustainable US biomass production potential that could support BECCS deployment. EFI has recently published a systematic literature review of the key opportunities and challenges associated with BECCS [2].

ORNL's work with EFI highlights opportunities for biomass supplies for BECCS that could be tapped while contributing to improved resource management and fulfilling sustainability criteria. Diverse estimates of potential biomass supplies are sensitive to the technical and economic parameters and assumptions of the specific studies cited. Discussion begins with supply estimates from [1], which are geospatially explicit, account for other market demands, and are supported by detailed descriptions of sustainability constraints and underlying economic and management assumptions. Next, sources that were not considered in BT16 but that are documented in recent literature (e.g., biomass derived from wildfire fuel reduction, cover crops, reclamation of land disturbed by mining) are discussed as additional potential supplies that merit further study. These feedstock categories were selected based on their potential to supply biomass without directly displacing current agricultural production or reducing soil carbon storage in the landscapes from which the feedstock is sourced. Supply estimates are followed by a discussion of sustainability factors and issues. The report emphasizes the need for secure markets to realize potential biomass collection and use. Finally, several more speculative estimates are discussed. Supplemental material provides additional details on the calculations and variables impacting sustainability.

RESULTS

Preliminary findings (Figure 1) show that an additional 1.4 billion annual dry Mg of sustainable biomass supply potential could be available, for a total of more than 2.4 billion Mg per year when combined with resources in BT16. Additional resources include wildfire fuels reduction in forests and shrublands, dedicated biomass crops on former mining and brownfield sites, use of winter season cover crops on farms, and managed biomass provision from the maintenance of right of ways (e.g., under power lines, along roads) on lands that require herbicides or other treatments to control growth or remove invasive species. Annual supply potential could be further increased with the adoption of genetically improved perennial crops, such as those being developed with federal support, that could conserve and build soil on marginal range and croplands.[2]

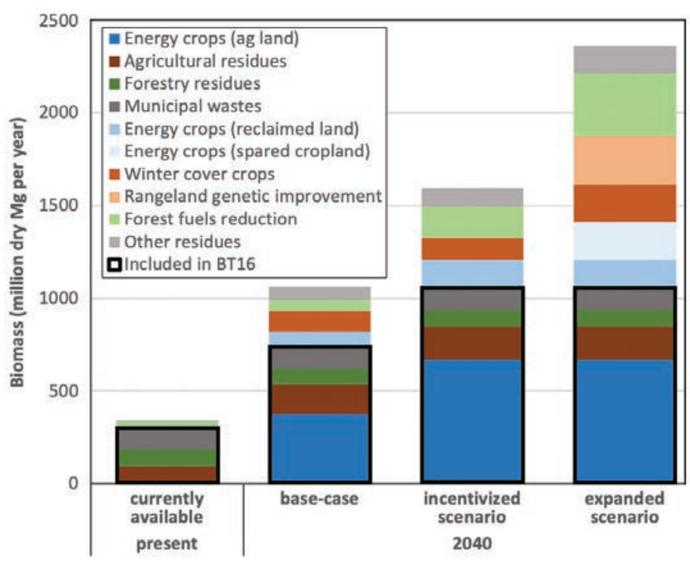

Figure 1. Biomass supply potentials in the contiguous United States from specified sources, present and in 2040. The black outline illustrates biomass potential quantified in the 2016 Billion Ton Study. Bars above the black outline represent other potential biomass sources assessed in this study. The base case represents a conservative estimate of well-documented resources that could be mobilized in the near term. The incentivized scenario reflects higher yields and advanced logistic systems. The expanded scenario includes additional supplies that merit more study, such as genetic improvements to enable economic biomass production on a small share of US rangeland and other marginal lands. All potentials represent biomass supplies that could be developed in compliance with sustainability criteria and while contributing to multiple sustainable development goals.

[1] Information on the BT16 study is available at https://www.energy.gov/eere/bioenergy/2016-billion-ton-report

[2] See https://federallabs.org/news/ornl-discovers-specific-gene-to-generate-better-crops to learn more about speculative feedstock sources that merit further study.

CONCLUSIONS

The data in Figure 1 illustrate significant potential for increased use of US biomass. However, several hurdles restrict the realization of sustainable biomass supply potentials including logistic and economic challenges, issues of public perception, legal and regulatory constraints, social implications of choices among land use options, and ongoing debates over the measurement and verification of sustainability. Specifically, biomass is inherently costly to collect, process, and mobilize, so potentials will remain unrealized in the absence of appropriate market incentives and some assurance of demand at competitive prices. Realization of sustainable biomass potentials requires investments to improve current natural resource management and supply chain logistics while contributing to social, economic, and environmental development goals. US potential remains underused because of biomass market barriers, including a lack of secure demand, risks for investors, and the availability of cheap fossil-based alternatives. Developing sustainable biomass supplies for BECCS will require investments to develop supply chains that have the following features:

- alignment with social and environmental goals;
- compliance with sustainability standards, ideally by using biomass that becomes available as a co-product of climate–smart land management;
- design that guides resource management practices that adapt to the changing climate and social and economic conditions;
- setting up of monitoring systems with site-specific targets using science-based indicators to measure and document change over time (i.e., criteria for sustainability must be relevant to local context);
- efficient production, collection, processing, and transport of inherently bulky, wet, and heterogenous biomaterials; and
- consistent delivery of feedstocks that meet clearly defined market specifications for quality.

IMPACT

Policy issues will also affect development of, and decision-making involved in, bioenergy strategies. With this in mind, members of ORNL's Environmental Sciences Division were recently featured in two workshops: "Rules of the Road for Bioenergy with Carbon Capture and Storage (BECCS) Deployment" and "Sowing the Seeds of a Negative-Carbon Future." These workshops were hosted by the EFI and targeted decision-makers focused on identifying and addressing barriers to using biomass supplies to advance a negative-carbon future. ORNL presented the preliminary results discussed in Figure 1.

The workshops highlighted technical issues critical to BECCS deployment, identifying several issues of note. First, the roundtable highlighted the potential value of biomass production for rural development and jobs but noted that there are challenges to overcome, such as assuring local benefits to communities and securing the investments required to improve resource management and supply chain efficiencies. Second, because of concerns about potential competition with other productive uses of land (and induced or indirect land use change [ILUC]), some strategies have aimed to incentivize the use of "wastes" as feedstock, but this approach must be considered with caution as it runs the risk of promoting more waste production. Third, lack of agreement on clear, practical, transparent, and widely adoptable methods for measuring carbon intensity and greenhouse gas emissions of feedstock production and use in BECCS is a major constraint. Other constraints include disagreements regarding best practices for modeling ILUC, time accounting for carbon removals and emissions, and the reference scenarios that define the alternative fate and conditions in the absence of the bioenergy option. Finally, understanding and demonstrating pathways toward "highest-value use of biomass" is a key goal, with ORNL research on locally led approaches being relevant because what constitutes the highest-value option depends on the context. A forthcoming EFI report will provide findings and conclusions from the workshops and related studies, as well as incorporate ORNL contributions to the assessment of sustainable biomass supplies.[3]

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[3] The EFI report will be available at https://energyfuturesinitiative.org/reports/

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