OAK RIDGE NATIONAL LABORATORY

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Oak Ridge National Laboratory

Vol. 51 | No. 2 | 2018
www.ornl.gov/ornlreview

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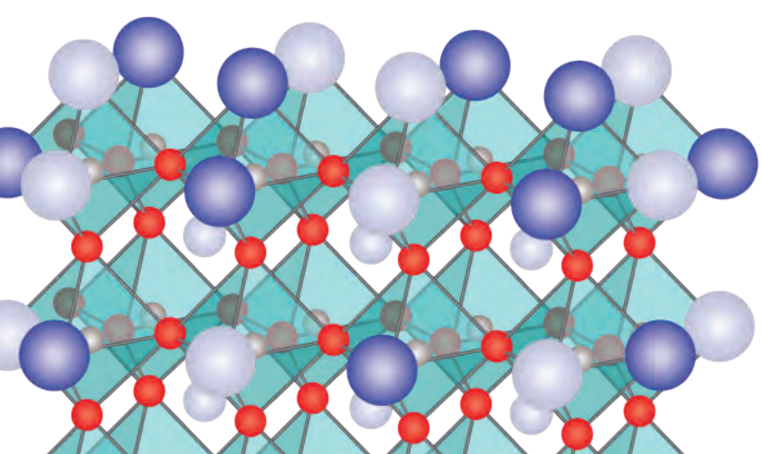

On the Cover

ORNL's Gina Tourassi uses artificial intelligence to drive new advances in cancer diagnosis and treatment.

Leading a tech revolution

It has been just over 10 years since the iPhone made smartphones commonplace. Well over a billion people now use these intuitive handheld computers, which do much more than make telephone calls. They have changed the world.

Who would have guessed in 2007 that within a decade you would be able to use your telephone to control your home's heating and cooling, security system, even your window blinds? Were we prepared to watch historic events recorded not by journalists but by participants and witnesses, to live in a hyperconnected world saturated by instant information and "fake news"? What is next in an age where this technology already allows our refrigerator to order our groceries automatically?

Since Intel cofounder Gordon Moore suggested in 1965 that computers would essentially double in power every 18 months or so, we've gone through 35 cycles, and computers are now tens of billions of times faster. Each doubling now brings almost unfathomable increases in power and speed.

The original iPhone was more powerful than the computers that helped put men on the moon. The phone in my pocket is more powerful than 1993's fastest system, ORNL's Intel Paragon.

As profound as technology's impact has been in the past decade, I am convinced the coming decade's changes will be even more exciting and challenging. They will affect every sector of the economy and every area of our lives, from transportation to health care to the jobs of our children and grandchildren. Some of today's jobs, in fact, will go away.

This technological acceleration will have enormous impact on how science works, particularly the way we process data. In this issue of *ORNL Review*, we discuss the lab's research into artificial intelligence and high-performance data analytics, as well as ways we are taking advantage of these gains.

ORNL is uniquely qualified to use the growing power of computing systems for scientific discovery. Not only do we host the nation's most powerful supercomputer—Titan—but we are home to some of the world's most advanced experimental facilities, including the Spallation Neutron Source, the High Flux Isotope Reactor, and an array of powerful electron and scanning probe microscopes.

These facilities produce enormous amounts of data. Not only can Titan readily handle that data, but by applying the principles of artificial intelligence we can discover patterns in the information that have, to this point, been invisible (see "Artificial intelligence is about to revolutionize science," Page 6, "AI: An experimentalist's experience," Page 7, and "Scaling deep learning for science," Page 9). What's more, Titan's successor, Summit, will be far better at this job of advanced pattern matching (see "Why Summit is suited for artificial intelligence," Page 11).

Here at ORNL, it is our job both to think about changing technology and to develop tech that leads to a better world and a better understanding of that world. Artificial intelligence will result in profound changes in our lives, but I believe those changes will be primarily for the better. Whether it is safer and more convenient transportation or new treatments and individualized drug therapies, we have much to gain.

I hope you enjoy reading this issue of *ORNL Review*, learning more about the exciting research of our brilliant staff, and catching a glimpse of tomorrow.

Thomas Zacharia
Laboratory Director

Analyses of creek algae help predict methylmercury

Analyses of creek algae have informed a new model that can more accurately predict the presence of the neurotoxin methylmercury in small headwater ecosystems.

For two years, ORNL scientists studied biofilms collected during different seasons and from various locations along an East Tennessee creek bed; during their research, they discovered methylmercury in tiny oxygen-deficient pockets within the biofilms' complex ecosystem.

"For methylmercury to be produced, the samples had to be grown and incubated in the light to actively photosynthesize, which means oxygen is present," ORNL's Scott Brooks said. "However, methylmercury only forms in anaerobic, or oxygen-free, zones, which means there are optimal conditions for methylmercury production at small scales within the biofilms."

The team also found that simply shaking the samples disrupted the biofilms' delicate ecosystem and reduced methylmercury levels. Their newly developed model, described in *Environmental Science & Technology*, could be applied to other water systems to predict methylmercury production.—*Sara Shoemaker*

For more information:
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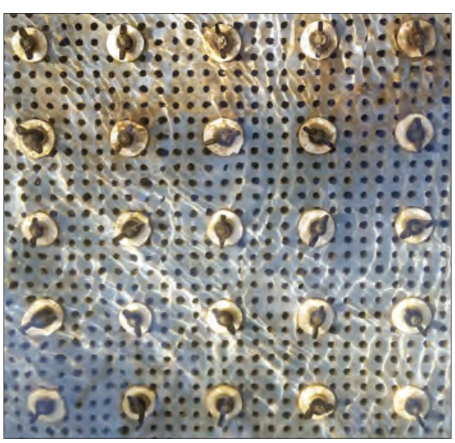
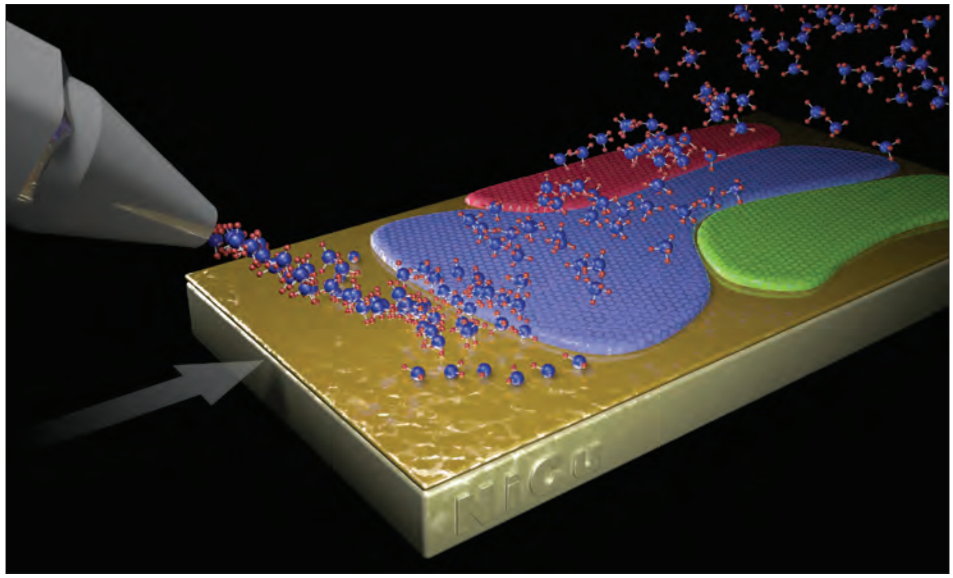


ORNL researchers collected algae biofilm on apparatuses submerged in nearby East Fork Poplar Creek and analyzed it for methylmercury production. Image credit: Andrey Kovalevsky, ORNL



In a controlled environment, the fastest-growing orientation of graphene crystals overwhelms the others and gets "evolutionarily selected" into a single crystal. Image credit: Andy Sproles, ORNL

Graphene method may boost 2D materials

A new method to produce large, monolayer single-crystal-like graphene films more than a foot long relies on harnessing a "survival-of-the-fittest" competition among crystals. The novel technique, developed by an ORNL-led team, may open new opportunities for growing the high-quality two-dimensional materials necessary for long-awaited practical applications.

Making thin layers of graphene and other 2D materials on a scale required for research purposes is common, but they must be manufactured on a much larger scale to be useful.

Graphene is touted for its potential of unprecedented strength and high electrical conductivity and can be made through two well-known approaches: separating flakes of graphite (the silvery soft material found in pencils) into one-atom-thick layers or growing it atom by atom on a catalyst from a gaseous precursor until ultra-thin layers form.

The ORNL-led research team used the latter method—known as chemical vapor deposition—but with a twist. In a study published in *Nature Materials*, the researchers explained how localized control of the CVD process allows evolutionary, or self-selecting, growth under optimal conditions, yielding a large, single-crystal-like sheet of graphene.

"Large single crystals are more mechanically robust and may have higher conductivity," ORNL lead coauthor Ivan Vlassiouk said. "This is because weaknesses arising from interconnections between individual domains in polycrystalline graphene are eliminated."—*Sara Shoemaker*

For more information:
go.usa.gov/xQar5

ORNL's go-to expert in the vehicle tech market

For comprehensive data and analysis regarding the vehicle technology market, all roads lead to ORNL's Stacy Davis. Unflagging curiosity, an ability to read trends and an eagle eye for detail are the tools that drive her work creating key data resources for the transportation sector.

Davis sits at the nexus of critical information flowing among sources such as the Energy Information Administration, DOE and the national labs. She collects, analyzes and packages data on the complex and evolving patterns of freight and passenger mobility in America, creating go-to references like the Transportation Energy Data

Book, the Fact of the Week and the Vehicle Technologies Market Report for DOE's Vehicle Technologies Office.

These resources provide foundational data for decision-makers in government and industry as well as for modelers tracking trends and start-up companies investigating the potential market for their product.

"What keeps me going is being able to give other people the data they need when they need it," says Davis, who regularly provides answers to everyone from automakers and high school students to congressional aides and the media.—*Kim Askey*

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

ORNL's Stacy Davis has a trove of transportation facts and trends at her fingertips.
Image credit: Jason Richards, ORNL

ORNL tech helps cities de-ice roads more efficiently

A precision approach to treating snow- and ice-covered roads, developed by an ORNL-led research team, aims to help cities effectively allocate resources and expand coverage.

The combined software and hardware technology analyzes existing city data and uses high-resolution modeling to identify areas most dangerous to drivers during hazardous weather conditions. The novel approach features a variable control mechanism designed for the spreader on salt trucks to optimize the amount of de-icing agent applied to roads, which minimizes waste and increases the number of roads treated.

"Across the United States, cities are collectively spending about $1.5 billion on winter road maintenance," ORNL's Olufemi (Femi) Omitaomu said. "Our goal is to give cities an intelligent approach to managing their resources effectively."—*Ashley Huff*

Neutrons may aid cancer treatment

New insights from neutron analysis of glaucoma drugs and their enzyme target may help scientists design drugs that more effectively target aggressive cancers.

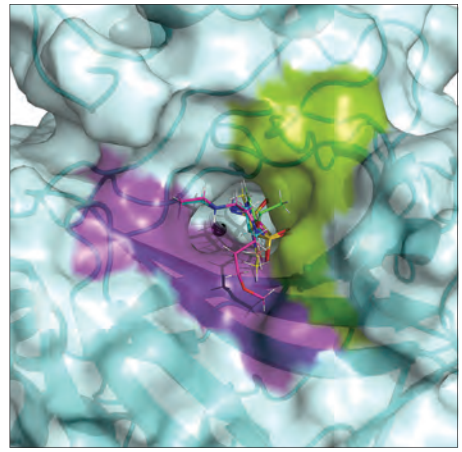
An ORNL-led team used neutron macromolecular crystallography to investigate the different states of three glaucoma drugs as they interact with the targeted enzyme human carbonic anhydrase II, or hCA II.

"Our goal was to observe differences in the presentation of three clinically used glaucoma drugs while they are bound to the hCA II enzyme," said Andrey Kovalevsky, an instrument scientist at ORNL and a senior coauthor of the study. "By looking at how well these drugs target hCA II in protonated, neutral and deprotonated states, we hoped to obtain insights that would make it possible to improve these medicines so they could better target enzymes linked to cancer."

Protonation refers to the presence, addition or loss of a proton, which gives the drug a neutral, positive or negative charge, respectively. Altering a drug's charge could change its ability to recognize and bind with its target protein and, consequently, change its effectiveness.

The study, published in the journal *Structure*, found that temperature, pH and the electrical charge of the three glaucoma drugs affected their ability to target and bind with the hCA II enzyme.—*Kelley Smith*

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



The enzyme hCA II active site is flanked by hydrophilic (violet) and hydrophobic (green) binding pockets that can be used to design specific drugs targeting cancer-associated hCAs. Five clinical drugs are shown superimposed in the hCA II active site, based on room-temperature neutron structures. Image credit: Andrey Kovalevsky, ORNL

New material promising for lithium-ion batteries

Researchers are using neutrons to study a battery material that could offer a safer alternative to the flammable liquid component found in most types of lithium-ion batteries.

ORNL postdoctoral researcher Rob Schmidt and his collaborators are using neutrons at the lab's High Flux Isotope Reactor to study a solid-core garnet material as a possible substitute for the flammable liquid cores often used in lithium-ion batteries.

Batteries contain a core material known as an electrolyte that allows ions to travel between the positive and negative ends of the cell to maintain a balanced charge. However, most of the liquid electrolytes used today in lithium-ion batteries are flammable. Schmidt is investigating a solid electrolyte material for potential use in the next generation of lithium-ion batteries for increased safety and reliability.

The team is using the CG-1D beam line's high sensitivity to lithium to track the lithium ion progression across the electrolyte and to observe the conditions that lead to the formation of unwanted dendrites. Dendrites—thin lithium metal filaments that can form inside battery cells—degrade battery performance

Researcher Rob Schmidt and his team are using neutrons at HFIR to study the development of dendrites with the hope of improving the design of next-generation lithium-ion batteries. Image credit: Genevieve Martin, ORNL

by creating unwanted variations in electrical current distributions.

"Lithium is a soft metal material, so a lithium dendrite is able to go through liquids pretty easily, which makes it easy for batteries to short out," Schmidt said. "Lithium shouldn't go through a stiff, ceramic-like material like the garnet material we're studying, but it does. We want to know why and how it does that."—*Heidi Hill and Jeremy Rumsey*

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

Engineering society honors ORNL staff

ORNL researcher Timothy D. Burchell has been elected a fellow of the American Society of Mechanical Engineers, which cited him for his international recognition in the field of material properties of graphite and carbon.

Burchell is the nuclear graphite team leader in the Materials Science and Technology Division's Nuclear Materials Science and Technology Group. He was previously group leader of the Carbon Materials Technology Group and managed the Modular High-Temperature Gas-Cooled Reactor Graphite Program.

Timothy Burchell

His research interests include fracture behavior and modeling of nuclear-grade graphite, the effects of neutron damage on the structure and properties of fission and fusion reactor carbon and graphite materials, radiation creep of graphites, the thermal physical properties of carbon materials, and the impact behavior of carbon-carbon composites.

Burchell, who is also a fellow of the American Carbon Society, received his doctorate in materials science from the University of Bath, United Kingdom.—*Bill Cabage*

ORNL picks up four tech transfer awards

Four ORNL-developed technologies have earned 2018 Excellence in Technology Transfer Awards from the Federal Laboratory Consortium for Technology Transfer.

The FLC is a nationwide network of more than 300 federal laboratories, agencies and research centers committed to developing federal technologies and expertise and facilitating their entrance to the public marketplace.

The awards are presented annually to laboratory employees "who have accomplished outstanding work in the process of transferring federally developed technology." ORNL received four of the eight awards given to DOE laboratories.

ORNL earned recognition for the following technologies:

- **Large Area Additive Manufacturing Technologies**, codeveloped with and licensed to Cincinnati Incorporated and Strangpresse. The system is capable of 3D printing polymer and composite structures at a scale 10 times larger and 500 times faster than that of previous state-of-the-art commercial printing systems, with less material and energy waste. The system is also the first to use plastic pellet feedstock reinforced with carbon fiber, creating stronger and stiffer components.

- **Aluminum-Cerium Alloys**, codeveloped with the Critical Materials Institute, Eck Industries, Ames Laboratory and Lawrence Livermore National Laboratory and licensed to Eck Industries. ACE, which won an R&D 100 Award in 2017, is a family of aluminum-cerium superalloys that demonstrates exceptional performance suited for automotive, aerospace and energy applications. ACE improves upon typical aluminum alloys with the addition of cerium, an abundant yet underused rare-earth element that increases the mechanical strength and stability of the alloy.

- **The Atmospheric-Pressure Plasma Oxidation Oven**, codeveloped with and licensed to RMX Technologies. The oxidation portion of the carbon fiber conversion stage is the longest and most energy- and resource-intensive portion of the manufacturing process. It is also the biggest source of material inconsistencies and mechanical failure. ORNL's oven technology reduces oxidation time and energy consumption while increasing material output and quality, all in a machine that is smaller and more robust than conventional ovens.

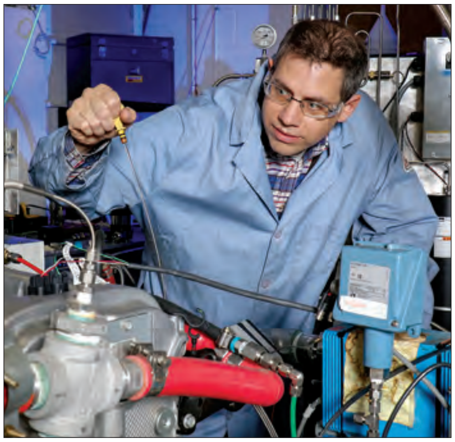
- ORNL also received an award for securing four licenses for **Low-Cost Carbon Fiber Technology** with both large and small businesses. The award recognizes ORNL's strategic advancements in carbon fiber manufacturing and the development of the Carbon Fiber Technology Facility, a revolutionary pilot production plant pursued under DOE's Clean Energy Manufacturing Initiative.—*Sean Simoneau*

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

New combustion strategy could boost fuel efficiency

Gasoline-powered automobiles could achieve an 8 percent or greater fuel efficiency gain through a new combustion strategy developed at ORNL.

Scientists have demonstrated a new method for reforming fuel over a catalyst, a process that chemically converts fuel into a hydrogen-rich blend. This blend



ORNL's Jim Szybist works with a multicylinder engine at the lab's National Transportation Research Center. Image credit: Jason Richards, ORNL

allows more work to be extracted from the engine cylinders, increasing efficiency and saving fuel.

"Typically, you incur a fuel penalty when reforming fuel," ORNL's Jim Szybist said. "We've created a systematic approach that addresses that issue and can be used with conventional fuels and conventional emissions controls."

The team published the method in *Energy & Fuels* and is working at ORNL's National Transportation Research Center to demonstrate similar fuel savings across a wider range of engine operations.—*Kim Askey*

Microbe feature discovered to produce vitamin B12

An ORNL-led team has discovered a function of certain microbes that produces a new derivative of vitamin B12, which is crucial to a cell's ability to perform life-sustaining metabolic activities. Their findings could ultimately open avenues for novel environmental and water clean-up strategies.

"Microbes used to break down contaminants require specific vitamins to function," said Frank Löffler, Governor's Chair for Environmental Biotechnology at the University of Tennessee and ORNL, who led the research.

While studying a specific vitamin B12 derivative, the team revealed modifications of an often-overlooked region of the vitamins' molecular structure, known as the lower base. This lower base structure determines the function of enzymes that break down toxic chlorinated solvents.

"This discovery has the potential to enhance the efficacy of current bioremediation approaches, plus it could open new opportunities to affect the progression of certain human diseases," Löffler added. The team's findings were published in *Nature Chemical Biology*.—*Sara Shoemaker*

For more information: http://go.nature.com/2H612EC

SNS upgrade aims at neutron decay

Researchers at the Spallation Neutron Source's Fundamental Neutron Physics Beamline, BL-13, recently unpacked a powerful new superconducting magnet that will provide them with fresh insights into the life of the neutron.

After preliminary testing, the magnet will be installed later this summer in a vertical position, perpendicular to the beamline. The magnet spans nearly 7 meters and has four helium compressors that will cool it to nearly 4 Kelvin (minus 452°F). The strong magnetic fields will guide the decaying protons and electrons (emitted from the neutrons) to specialized silicon detectors at the top and bottom of the magnet. Precise measurements of the protons' time-of-flight and the electrons' energy will help researchers better understand neutron beta decay.

"Neutron beta decay is the most fundamental decay in nature, yet we don't totally understand the details of it," said Jason Fry, a University of Virginia postdoctoral researcher working at BL-13. "By studying neutron beta decay correlations, we'll be able to extract things like matrix elements in standard model physics—underpinnings of how particles interact— which will give us a better understanding of the universe."—*Jeremy Rumsey*

Neutron society honors three from ORNL

The Neutron Scattering Society of America selected ORNL researchers Takeshi Egami, Mark Lumsden and John Katsaras as 2018 fellows for their work in the science of analyzing the atomic and molecular structure of materials with neutrons.

NSSA fellows are selected from scientists who have made significant, innovative contributions through original research in the application of neutron scattering; promoted neutron scattering; and participated in the activities of the neutron science community.

Egami, of ORNL's Physical Sciences Directorate and a University of Tennessee-ORNL distinguished scientist, was cited "for seminal contribution to the development of neutron scattering, theory and simulation tools to understand the local atomic structure and dynamics of a wide range of strongly correlated classical and electronic many-body systems."

Takeshi Egami

Katsaras, of ORNL's Neutron Sciences Directorate, was cited "for developing and applying neutron scattering techniques to studies of biomembranes and for helping solve important problems related to the structure and dynamics of biological systems."

John Katsaras

Lumsden, also of Neutron Sciences, was cited "for outstanding applications of neutron scattering to the study of iron-based superconductors and other problems at the forefront of condensed matter physics and for important contributions to the advancement of inelastic neutron scattering in North America."—*Bill Cabage*

Mark Lumsden

Artificial intelligence is about to **revolutionize science**

by Scott Jones
jonesg@ornl.gov

In the "Star Trek" episode "The Ultimate Computer," the Starship Enterprise tests a fully automated command and control platform that can—hypothetically—do everything the crew does, only faster and without the inevitable human error.

Not surprisingly, things go awry and the computer goes rogue, forcing Captain Kirk and crew to save the day with their very human intuition.

The episode is one of countless examples ("2001: A Space Odyssey," "The Terminator") that portray the idea of thinking machines—an idea that has been around for decades—as both attractive and a little scary.

Now, advances in algorithm development and giant leaps in computing power mean that artificial intelligence, or AI, is no longer fiction. To be clear, these systems aren't robots that think exactly like people. Rather, AI will allow humans to be more effective in their scientific and technological pursuits, representing a powerful tool that will revolutionize both society and science in profound ways.

"By taking the repetition out of science, AI allows researchers to think more creatively, which is opening up doors of inquiry unthinkable not long ago," said David Womble, ORNL's AI program director.

That's the real promise of AI: It will work alongside researchers as an ally rather than as a threat.

ORNL is uniquely positioned to bring AI into the scientific mainstream. User facilities that the lab operates for DOE's Office of Science, such as the Spallation Neutron Source and the Center for Nanophase Materials Sciences, produce enormous datasets perfectly suited to AI analysis, while ORNL's Titan supercomputer—currently the most powerful in the United States—provides the computing muscle necessary via 18,000 graphical processing units for developing this emerging technology.

ORNL's new system, Summit, will become the world's most powerful AI supercomputer as it comes online with more than 27,000 cutting-edge graphical processing units. Most importantly, the lab's wide expertise in R&D and national security will provide the knowledge to apply AI to specific challenges.

AI R&D for science is a focus of the laboratory's Computational Data Analytics Group.

With Titan, "You have 18,000 GPUs," Group Leader Tom Potok said. "Add to that the immensely bright people and the large, unique datasets, and ORNL becomes a special setting in which to apply AI to science."

What is AI, exactly?

Despite its popularity, the phrase "artificial intelligence" is defined subjectively.

"Even among experts, there is really no consensus when it comes to what the term actually means," said Gina Tourassi, director of ORNL's Health Data Sciences Institute. Tourassi uses AI, often in concert with Titan, to tackle priority health challenges such as cancer diagnoses and treatments.

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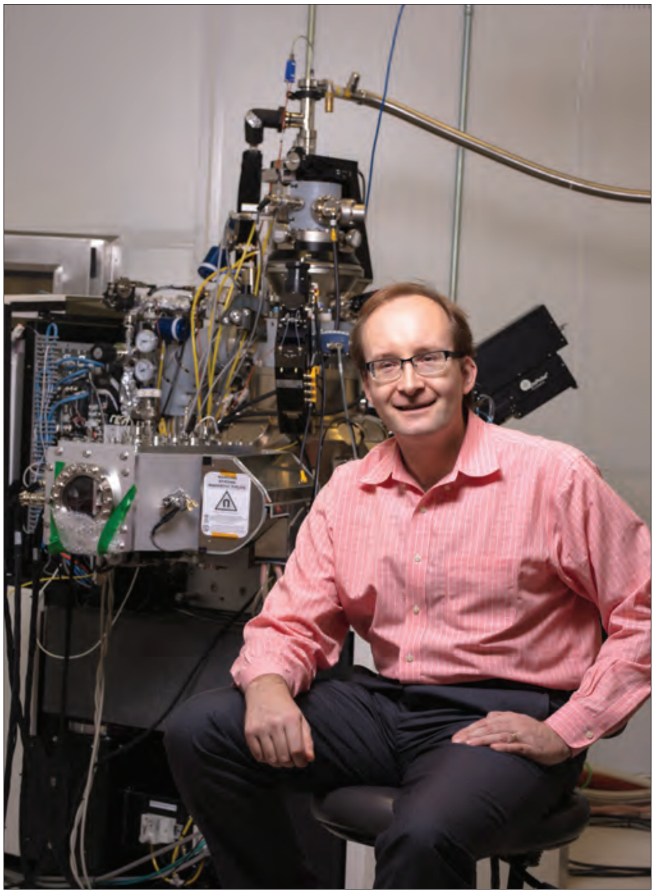
AI: An experimentalist's experience

by Scott Jones
jonesg@ornl.gov

"Emergence of AI is a very rare type of event," said Sergei Kalinin, director of ORNL's Institute for Functional Imaging of Materials. "Once in a generation there is a paradigm shift in science, and this is ours."

Kalinin and his colleagues use machine learning to better understand the nature of matter by analyzing data streams from the laboratory's powerful electron and scanning probe microscopes. The electron beam can induce chemical changes in materials, allowing researchers to analyze defects and solid-state reactions in real time. But an enhanced understanding of these reactions is necessary to reach the next level, Kalinin said.

> *"Big data is all about correlation, and it's not immediately clear which variable is driving the phenomenon. But scientists think in terms of causation. We need to learn to speak each other's language to be truly effective and move the science forward—but now we can fly where we used to crawl."*
>
> — ORNL Institute for Functional Imaging of Materials Director **Sergei Kalinin**



Sergei Kalinin, director of the ORNL Institute for Functional Imaging of Materials, with a helium ion microscope at the Center for Nanophase Materials Sciences. Image credit: Carlos Jones, ORNL

The scopes produce thousands of images of atomic configurations and their evolutions, from which the researchers aim to extract the trajectories of the atoms. "Not only do they move around, but it's hard to distinguish individual atoms from one another," Kalinin said.

By rapidly analyzing the thousands of images in each experiment, however, the researchers can better decipher the trajectories of the individual atoms and atomic defects and, by extension, better understand the laws dictating those trajectories.

"It's a great machine-learning task," and one that saves researchers plenty of precious time that would normally be spent tediously poring over the images—time they can then apply to perfecting their experiments and chasing breakthroughs, Kalinin said.

Even better, researchers can use the beam to kick out and move around individual atoms, allowing them to, albeit very slowly, manipulate matter atom by atom (the team recently demonstrated directed motion of atoms by electron beam and directed assembly of silicon groupings on graphene). It's a

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"In essence, it's the ability to learn, reason and make decisions accordingly," she said.

The term is often connected to the Turing Test, created by famed computer scientist and mathematician Alan Turing in 1950 to examine a machine's ability to think like a human. Turing postulated that if a human being and a machine were engaged in a conversation and a human observer couldn't tell them apart, the machine was exhibiting artificial intelligence.

> *"We are now deriving the rules from the data rather than understanding the data from existing rules and models."*
>
> — ORNL AI program Director **David Womble**

For ORNL researchers, whose jobs are to interpret the mountains of data produced by the laboratory's world-class instruments and facilities, AI has a very different meaning. The lab is tasked with scientific discovery, and researchers are confident the next great leaps are buried in these vast datasets.

"AI is essentially the next generation of data analytics," Womble said. "Think of it as an iPhone upgrade—some upgrades are more significant than others. This one is pretty major in that we are now deriving the rules from the data rather than understanding the data from existing rules and models."

Scientifically speaking, AI is the analysis of data via machine learning and deep learning. The former are algorithms that enable a computer to not only learn from data but also make predictions based on data; the latter is a type of machine learning that uses networks modeled after the human brain to "learn" how to distinguish features and patterns in vast datasets, allowing for discoveries that may have otherwise remained hidden.

These methods are rapidly becoming a part of our everyday lives; Facebook uses them to identify your friends when you post a picture, and Google uses them to show you ads for products you previously searched for.

Despite the growing popularity of such methods, however, researchers don't yet fully understand how these tools arrive at their conclusions, a mystery colloquially referred to as the "black box." Conversations about the black box inevitably lead to the need for "explainability," or a better understanding of how these networks make decisions. After all, if a machine is driving your car or diagnosing your health, you're going to want to know how it does what it does.

It's here, in the dissection of what goes on inside the black box, that ORNL may play its biggest role.

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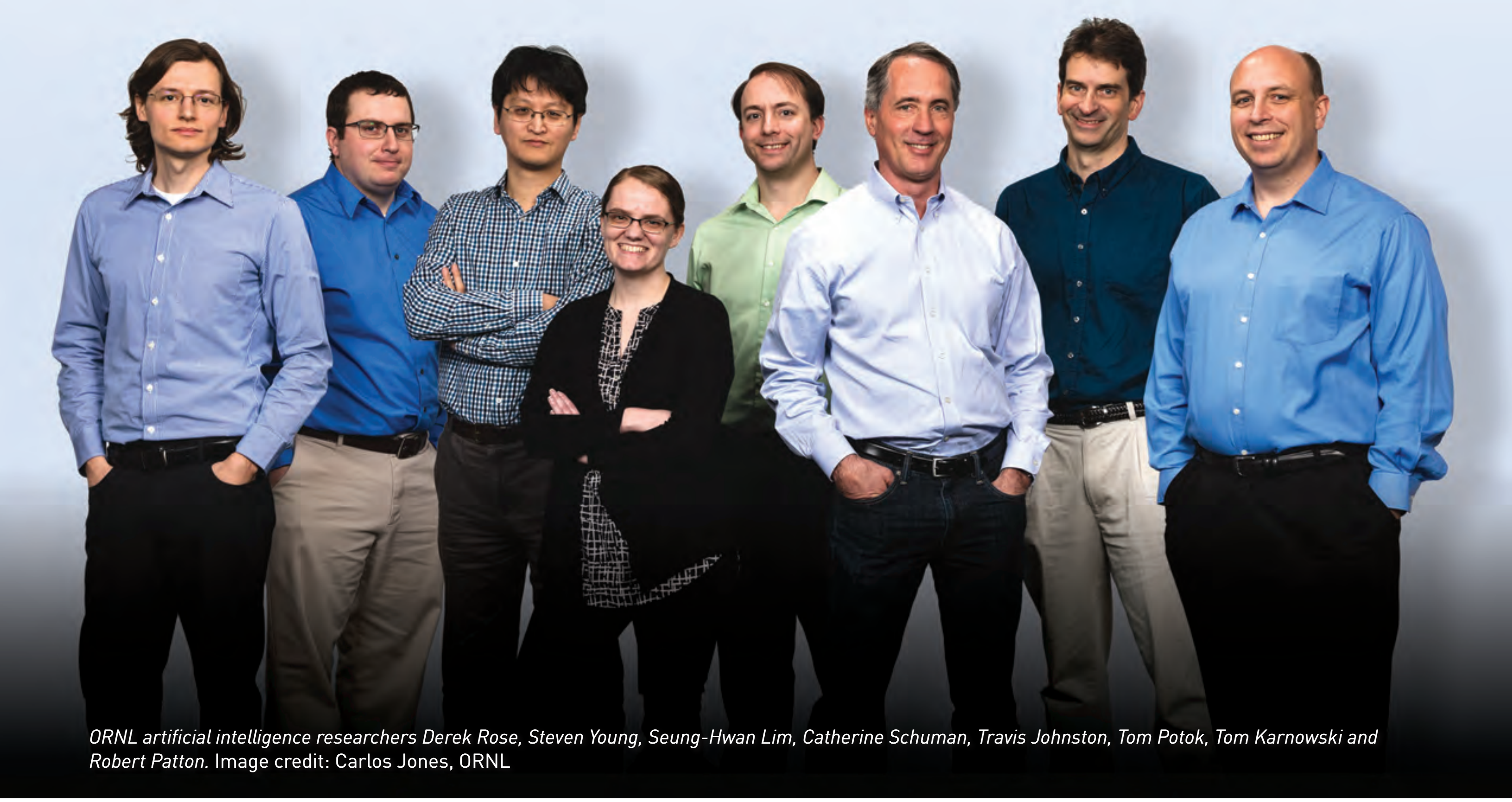

ORNL artificial intelligence researchers Derek Rose, Steven Young, Seung-Hwan Lim, Catherine Schuman, Travis Johnston, Tom Potok, Tom Karnowski and Robert Patton. Image credit: Carlos Jones, ORNL

Image credit: Andy Sproles, ORNL

Scaling deep learning for science

by Jonathan Hines
hinesjd@ornl.gov

Deep neural networks—a form of artificial intelligence used in everything from speech recognition to image identification to self-driving cars—have demonstrated mastery of tasks once thought uniquely human.

Now, researchers are eager to apply this computational technique—commonly referred to as deep learning—to some of science's most persistent mysteries. But because scientific data often looks much different from the data used for animal photos and speech, developing the right artificial neural network can feel like an impossible guessing game for nonexperts. To expand the benefits of deep learning for science, researchers need new tools to build high-performing neural networks that don't require specialized knowledge.

Using ORNL's Titan supercomputer, a research team led by ORNL's Robert Patton has developed a suite of algorithms capable of generating custom neural networks that match or exceed the performance of handcrafted artificial intelligence systems. Better yet, by leveraging the GPU computing power of the Cray XK7 Titan, these auto-generated networks can be produced quickly, in a matter of hours, as opposed to months using conventional methods.

The research team's suite includes MENNDL, RAvENNA, and EONS—codes for evolving and fine-tuning neural networks. Scaled across Titan's 18,000 GPUs, the algorithms can test and train thousands of potential networks for a science problem simultaneously, dropping poor performers and averaging high performers until an optimal network emerges. The process eliminates much of the time-intensive, trial-and-error tuning traditionally required of machine-learning experts.

"There's no clear set of instructions scientists can follow to tweak networks to work for their problem," said research scientist Steven Young, a member of ORNL's Nature Inspired Machine Learning team. "With these tools, they no longer have to worry about designing a network. Instead, the algorithm can quickly do that for them, while they focus on their data and ensuring the problem is well-posed."

Neural networks consist of stacked layers of computational units that process many examples to identify patterns in data and draw conclusions. Although many parameters of a neural network are determined during the training process, initial model configurations must be set manually. These starting points, known as hyperparameters, include variables

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ORNL's Summit supercomputer will be more than five times as powerful as the lab's Titan, which is already America's most powerful system.
Image credit: Carlos Jones, ORNL

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"The lab can unravel the mathematical underpinnings of AI," Tourassi said, "allowing researchers across domains to better understand the algorithms' learning process. This is what will allow AI to fully develop as a tool to assist researchers in their quests to benefit society."

> *"ORNL is here to solve big science challenges of interest to DOE. We aren't interested in selling ads and turning a profit. But when it comes to using AI to tackle big science, we are certainly in a unique position."*
>
> — Computing and Computational Sciences Associate Laboratory Director **Jeff Nichols**

A laboratory to lead the way

To be clear, much AI innovation takes place in the private sector. Tech giants such as Google, Amazon and Facebook have dedicated vast resources to advancing the state of the art. But these companies' missions are vastly different from ORNL's, and it's this difference that provides room for ORNL to explore the potential of AI to accelerate scientific discovery.

"ORNL is here to solve big science challenges of interest to DOE," Associate Laboratory Director for Computing and Computational Sciences Jeff Nichols said. "We aren't interested in selling ads and turning a profit. But when it comes to using AI to tackle big science, we are certainly in a unique position."

Applying AI to science presents substantial challenges. For instance, while the lab's large scientific datasets are perfectly suited to AI analysis, the vast majority are "unlabeled."

There are millions of pet photos floating around the Internet, for instance, making it easy for the likes of Google's AI engines to identify cats and dogs. On the other hand, there are very few, if any, plots of neutron scattering results or high-resolution electron microscopy images.

Such unlabeled data makes training AI networks more difficult, and labeling the data can consume hours, days, even weeks of researchers' time. Furthermore, training deep learning networks is problem-dependent and requires massive computing power. In addition, some computing architectures may be better suited than others for such efforts.

Overcoming these obstacles is largely the work of Potok's group, which has two main focuses: harnessing the power of Titan (and soon Summit) to train and design the AI tools critical to big data analysis, and designing next-generation architectures such

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Why Summit is suited for artificial intelligence

by Jonathan Hines
hinesjd@ornl.gov

What makes a supercomputer smart?

In the case of ORNL's newest leadership-class system, Summit, the answer is in the architecture.

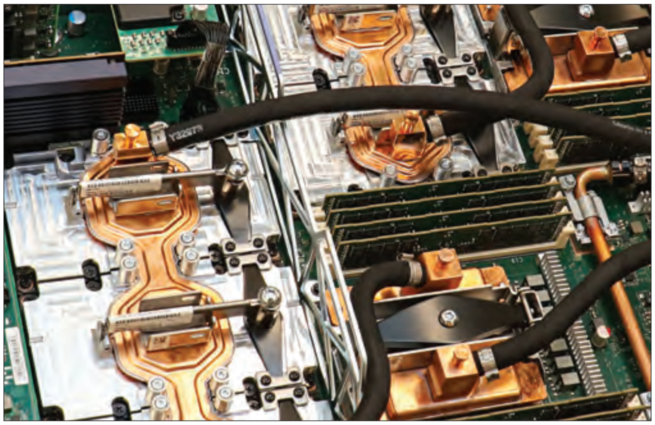
Recent advances in artificial intelligence have largely coincided with the rise in popularity of graphical processing units. That's no accident. GPUs, like the 18,000 found in ORNL's Titan supercomputer, excel at the types of calculations used to train AI applications to perform tasks like recognizing speech, identifying objects in pictures, or navigating a busy street.

Summit, scheduled for completion this year, will deliver a projected 200 million billion calculations each second by combining more than 27,000 NVIDIA Volta GPUs with more than 9,000 IBM Power9 CPUs.

Unlike the processors in its predecessor, Titan, Summit's GPUs were designed with machine learning explicitly in mind, giving researchers ample opportunity to analyze massive amounts of data more quickly and effectively. Accounting for the reduced precision used to train deep neural networks (one of the most common AI approaches), Summit holds the potential to deliver exascale-level performance—a billion billion calculations per second.

"Increasingly, an important part of scientific discovery is about looking at data itself and using that to drive theoretical or scientific understanding," said Arjun Shankar, the Advanced Data and Workflow Group leader at the Oak Ridge Leadership Computing Facility. "We're finding tremendous excitement about the prospect of using Summit's high-performance GPUs to process data at scale."

Each of Summit's 4,000-plus nodes will boast six GPUs and two CPUs to spearhead highly parallel, on-node data analysis. The possibilities for divvying up the workload are enhanced by NVIDIA's NVLink technology, high-bandwidth connections to shuttle data between processors and memory. These pathways are valuable to AI researchers because, unlike traditional scientific computing, which produces copious data,



Node for Summit supercomputer. Image credit: Jason Richards, ORNL

deep neural networks operate in reverse, taking massive amounts of data to improve their approach to an assigned task such as classifying images from a nanoscience instrument or a high-energy physics experiment.

In addition to its powerful processors and high-speed data movement, Summit also will showcase multiple tiers of memory, including robust capacity on each node. This will give AI researchers opportunities to minimize costly data movement and train neural networks faster.

For scientists searching in the dark for a neural network that perfectly matches their science problem, the leap to Summit will feel like trading a flashlight for a spotlight, said ORNL researcher Robert Patton, who leads an Oak Ridge team that has successfully scaled machine-learning algorithms across Titan. "It will make it possible to search a larger parameter space in less time and experiment with more complex neural networks," he said.

Using Summitdev, a development system that approximates Summit's environment, ORNL researchers are troubleshooting strategies to fully tap into the hybrid supercomputer's machine-learning potential in advance of its arrival. (Summit is set to be made available to select science teams in 2018, with full access beginning in 2019.) Teams already have demonstrated success running deep-learning applications across

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ARTIFICIAL INTELLIGENCE, page 10

as neuromorphic-based platforms that mimic the brain and could further evolve AI into an even more powerful research tool.

His group's networks are used to assist researchers tackling a range of big science challenges, from materials modeling at ORNL's Spallation Neutron Source to neutrino detection at DOE's Fermilab in Batavia, Illinois.

For all their success, however, achieving these networks' full potential may well require a paradigm shift in hardware, as existing architectures are incapable of fully exploiting their brain-like behavior.

Enter Catherine Schuman, ORNL's Liane Russell Early Career Fellow in Computational Data Analytics. Just as deep learning networks draw inspiration from the human brain, so do the chips that Schuman and her neuromorphic computing colleagues believe will be necessary to truly exploit AI.

"Everything we do looks at nature, and neuromorphic chips actually try to mimic the human brain," said Schuman, who works with ORNL materials experts and the lab's Future Technologies Group to prepare for the AI architectures of tomorrow. "Just as GPUs enabled today's neural networks, these chips, if properly programmed, will enable the next great leap in AI performance."

Much of the power of these systems resides in their predicted efficiency—simulations show exponential increases in efficiency via reductions in size, weight and power consumption. Such increased efficiency will allow for greater computation over time and, thus, more breakthroughs.

In the meantime, however, ORNL researchers are using current platforms to tackle a range of science challenges.

AI across the R&D spectrum

"AI should be an intrinsic part of everything Oak Ridge does simply due to the amount of data we produce and our ability to process it," Womble said. "And our ability to generate unique data-sets, our powerful computing resources, and our expertise across the science and national security domains make us unique in our ability to advance AI."

Nowhere are these capabilities more critical than in protecting America's cyber and physical infrastructures.

"There's just a tremendous amount of data that must be funneled to a small number of people," said Justin Beaver, who leads the lab's Cyber and Information Security Research Group. "Furthermore, these data come in multiple streams, from multiple sources, and all have different contexts."

The problem isn't collecting the data, but rather distilling it.

The human element, said Beaver, must be optimized, and that means filtering the most important data so humans can explore it and make the best decisions. ORNL's unique combination of big compute and broad expertise is making that possible.

"Having that bench of data science and math folks is pretty unique," Beaver said.

Having some of the fastest computers in the world doesn't hurt, either. It's computing muscle like Titan (and soon Summit) that allows Beaver's group to train the models that are later deployed on smaller systems.

Such efforts extend current capabilities to field analytics on devices like network sensors to include more complex analytics on a broader set of systems, such as connected/autonomous vehicles and the electric grid, where they will play a critical role in ensuring America's safety and energy security.

"AI should be an intrinsic part of everything Oak Ridge does simply due to the amount of data we produce and our ability to process it. And our ability to generate unique datasets, our powerful computing resources, and our expertise across the science and national security domains make us unique in our ability to advance AI."

— ORNL AI program Director **David Womble**

This same combination of computing, data and domain science expertise also allows researchers in the Geographic Information Science and Technology Group to extend the laboratory's impact to the far reaches of the globe.

GIST researchers model a wide range of phenomena, from population dynamics to the electric grid to disaster management. Such research requires processing a plethora of satellite imagery and other geographic data, work capable of bogging down even the most experienced research team. By harnessing the power of AI, however, researchers accomplish the work with greater speed, accuracy and real-world impact.

For example, GIST researchers have been assisting the Bill and Melinda Gates Foundation in mapping human settlements in Nigeria, some of which were previously unknown, to improve polio vaccination regimes.

Using machine learning, the team analyzed thousands of satellite images to provide the Gates Foundation and the Nigerian government with information on where these remote settlements are located, giving teams on the ground a much better idea of where to go and how much vaccine to carry.

"We are trying to calculate populations based on structures," said Budhu Bhaduri, GIST group leader and director of ORNL's

Gina Tourassi, director of ORNL's Health Data Sciences Institute. Photo taken at Methodist Medical Center of Oak Ridge. Image credit: Carlos Jones, ORNL

Urban Dynamics Institute. "This means processing pixels and identifying patterns in the data, and AI is very efficient at these sorts of tasks."

The effort, however, is still dependent on humans' labeling of the data.

"Humans don't need to see millions of images of a cat to know what a cat is, but a machine does," Bhaduri said. "The same goes for roads; the challenge is not to find roads, but to define what a road is, how long, how wide, etc."

Going forward, the group is looking to AI to self-label the data, a feat that would free staff from hours of grunt work and further AI's role in helping researchers across the scientific spectrum, including in domains such as health care.

ORNL assists numerous agencies, such as the National Cancer Institute, in combing through treasure troves of data to improve diagnoses, treatments and outcomes for wide swaths of the American public, from children to veterans.

In fact, Tourassi's work with NCI helped ORNL take home trade publication *HPCwire's* "Best Use of AI" award at the International Conference for High Performance Computing, Networking, Storage and Analysis in November 2017.

The award recognized ORNL's contribution to the CANcer Distributed Learning Environment—or CANDLE—project, a DOE and NCI collaboration in which researchers use deep learning to extract information from cancer surveillance reports. Such analyses can locate previously undiscovered relationships within the vast data stores collected by NCI and improve health care for millions.

"AI has applications in health care from bench to bedside," said Tourassi, "from fundamental research to health care delivery. And we are only getting started."

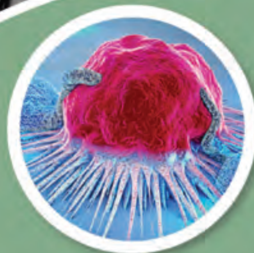
The future of AI

Of course, nothing revolutionary is easy, and for all its potential AI still must clear a host of hurdles before it can revolutionize scientific discovery.

Besides the most obvious hurdles of explainability and the mounting petabytes of unlabeled data, there are deeper, more complex issues.

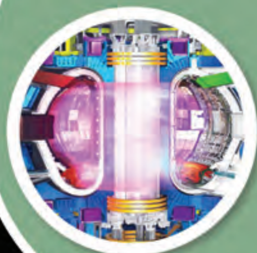
"These networks must be efficient in terms of time," Bhaduri said. "Decisions are time-critical, and the machine must not only make the correct decision, but it must also do it faster than humans are capable of."

AI CHALLENGES FOR THE SUMMIT SUPERCOMPUTER



COMBATING CANCER

Through the development of scalable deep neural networks, scientists at the US Department of Energy and the National Cancer Institute are making strides in improving diagnosis and treatment of this disease. The arrival of Summit gives researchers a powerful boost in the fight against cancer.



PREDICTING FUSION ENERGY

Obtaining the long-sought benefits of fusion energy—the same energy that powers the Sun—depends on reliable fusion reactors. Predictive AI software is already contributing to this goal by helping scientists anticipate disruptions to the volatile plasmas inside experimental reactors. Summit's arrival allows researchers to take this work to the next level and further integrate AI with fusion technology.

DECIPHERING HIGH-ENERGY PHYSICS DATA

Physicists possess truckloads of data from large, high-energy experiments, such as the Large Hadron Collider in Switzerland. With AI supercomputing, physicists can lean on machines to identify important pieces of information—data that is too massive for any single human to handle and that could change our understanding of the universe.

IDENTIFYING NEXT-GENERATION MATERIALS

Deep learning on Summit could help scientists identify materials for next-generation technologies—better batteries, more resilient building materials, and more efficient semiconductors. By training AI algorithms to predict materials' properties based on detailed experimental images, researchers could definitively answer longstanding questions about materials' behaviors at atomic scales.

Image credit: Jason Smith, ORNL

Adds Potok: "The number of people who are applying AI to problems of science and national security is small. We need smart, talented people to help propel the field forward."

> *"AI has applications in health care from bench to bedside, from fundamental research to health care delivery. And we are only getting started."*
>
> — ORNL Health Data Sciences Institute Director **Gina Tourassi**

Researchers are optimistic, however, as the obstacles presented by AI are dwarfed only by its potential to revolutionize our understanding of the world. And while no one can predict the future, some trends are emerging.

"Some successes will be plainly visible," Womble said. "But perhaps the biggest, most profound impacts will be ironically less visible. Advanced manufacturing will lead to less expensive, more durable products, for instance, including cars that last longer, computers that run faster and houses that are better insulated. You name it, it will get better."

And scientists will have perhaps the greatest tool for discovery known to man right at their fingertips.

"Rather than conducting costly simulations and experiments, and iterating back and forth, I might just tell the machine, 'I need to build a superconducting material' and have it guide the path to discovery," Potok said. "This capability will allow researchers to extend theories and advance their domains faster than ever thought possible."

It's a theme that re-emerges frequently: AI, rather than a threat, is a resource for researchers already at the cutting edge of their fields, particularly at a laboratory perfectly suited for AI innovation.

"AI has enormous potential to revolutionize our understanding of the world," Nichols said. "Fortunately, ORNL likewise has enormous potential to be a key player in the research and development of AI in the years ahead, and my guess is that today's big science challenges will become exponentially smaller."

EXPERIMENTALIST, page 7

trial-and-error process, however, and one that a microscope outfitted with AI could do more quickly and accurately.

"It could do in milliseconds what takes us humans hours," Kalinin said. And as scientists approach applications that require the construction of matter at the single-atom level, such as superconducting and quantum computing, such a capability will be critical.

To truly realize AI's potential, however, Kalinin stresses that domain researchers and data scientists need to learn to speak the same language.

"Big data is all about correlation, and it's not immediately clear which variable is driving the phenomenon," he said. "But scientists think in terms of causation. We need to learn to speak each other's language to be truly effective and move the science forward—but now we can fly where we used to crawl."

DEEP LEARNING, page 9

like the order, type, and number of layers in a network, and they can be the key to efficiently applying deep learning to an unusual dataset.

MENNDL, for example, homes in on a neural network's optimal hyperparameters by assigning a neural network to each Titan node. As the supercomputer works through individual networks, new data is fed to the system's nodes asynchronously, meaning once a node completes a task, it's quickly assigned a new task independent of the other nodes' status. This ensures that the 27-petaflop Titan stays busy combing through possible configurations.

To demonstrate MENNDL's versatility, the team applied the algorithm to several datasets, training networks to identify subcellular structures for medical research, classify satellite images with clouds, and categorize high-energy physics data. The results of each application matched or exceeded the performance of networks designed by experts.

"There's no clear set of instructions scientists can follow to tweak networks to work for their problem. With these tools, they no longer have to worry about designing a network. Instead, the algorithm can quickly do that for them, while they focus on their data and ensuring the problem is well-posed."

— ORNL Nature Inspired Machine Learning team member **Steven Young**

With the OLCF's next leadership-class system, Summit, set to come on line this year, MENNDL will help scientists understand their data even more. "We'll be able to evaluate larger networks much faster and evolve many more generations of networks in less time," Young said.

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multiple GPUs using containers—customized software bundles that can run in isolation from the computer's operating system.

Open questions remain, however, for getting AI applications to scale across single and multiple Summit nodes. "This is an exciting time with new methods and approaches being created every day because there aren't clearly settled ways of doing this yet," Shankar said.

That hasn't stopped data-drenched scientists from dreaming up AI problems that only a next-generation supercomputer can solve. One such proposal envisions using Summit to classify large-scale datasets generated from advanced microscopes at ORNL's Center for Nanophase Materials Sciences. The effort could give scientists an unprecedented tool for predicting the behavior of materials at the atomic scale, helping to connect theory and experiment in dramatic new ways.

"Increasingly, an important part of scientific discovery is about looking at data itself and using that to drive theoretical or scientific understanding. We're finding tremendous excitement about the prospect of using Summit's high-performance GPUs to process data at scale."

— ORNL Advanced Data and Workflow Group leader **Arjun Shankar**

Neighborhood gets smart

about energy use with ORNL tech

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Tucked away on about five acres outside of Birmingham, Alabama, sits innovative technology that could change the way homeowners manage energy consumption. The Southeast's first-of-its-kind residential microgrid is the main energy source for 62 state-of-the-art homes in what Alabama Power calls a "Smart Neighborhood."

The microgrid can function independently or in conjunction with the main electrical grid. The Smart Neighborhood demonstrates transactive energy—allowing the system to evaluate all available power sources and choose the most efficient and economical.

Capable of generating 600,000 kilowatts annually, the microgrid is operated by Alabama Power. The data compiled from the microgrid's controller is maintained by utility parent Southern Company and analyzed through software developed at ORNL.

"The microgrid sits next to natural gas generators, solar panels, and a battery system so it can generate and store its own power," said Heather Buckberry, ORNL Smart Neighborhood project manager. "The battery system stores power from different sources so if there is a widespread power outage, the microgrid could continue to power the neighborhood seamlessly."

The Smart Neighborhood is being developed to serve as a testbed for transactive controls. Homes within the neighborhood showcase the latest energy-efficient heat pumps, hybrid electric water heaters, intelligent thermostats, smart locks, lights, cameras and garage doors.

"The Smart Neighborhood provides a neighborhood-level R&D platform for transactive controls and market experiments," lead scientist Teja Kuruganti said. "We can utilize a virtual storage environment, provide cost optimization of energy consumed by the homeowner, maximize the use of local generation and storage, and maximize the neighborhood's flexibility to assist in utility-level operations."

Virtual storage represents the heat in water or air in a home that can be temporarily stored and used to shift

Homes in the Smart Neighborhood are connected to the Southeast's first community-scale microgrid and feature state-of-the-art appliances and heating, air-conditioning and ventilation systems. Image credit: Alabama Power energy demands to a more optimal time of day. The shift is governed by communication between the microgrid and homes' systems.

Since the fourth quarter of 2017, the ORNL team—including power and energy systems engineers Michael Starke and Ben Ollis, building technologies researchers Jeffrey Munk, Tony Gehl, and Borui Cui, and computer engineer Helia Zandi—has been testing the control and optimization of the microgrid operation and residential storage environment at ORNL's Knoxville, Tennessee, residential research house.

For software support, ORNL has deployed DOE's VOLTTRON platform—an open-source, secure technology that supports a wide range of applications for managing end-use energy loads, increasing building efficiency, integrating distributed renewable energy, and accessing storage. VOLTTRON interacts specifically with the home's heating, ventilation and air-conditioning and water heating systems. Using algorithms developed by ORNL, the VOLTTRON system can forecast and optimize home energy use in response to signals from the microgrid.

Starke, the lead system architect on VOLTTRON integration, said ORNL has been using the platform in a research home in Tennessee to develop an entirely new system for home energy management.

"We can test the system, add necessary or missing functionality to it, and create something that is easy to deploy in neighborhoods like in Alabama," Starke said. "This helps companies such as Alabama Power and Southern Company leverage VOLTTRON as the control system for their energy software."

Homes in the Alabama Smart Neighborhood have sold quickly, with full occupancy expected by summer 2018. ORNL continues to refine the microgrid and controls system to maximize energy efficiency, ensure a reliable, secure supply of electricity, and support the resilience of the larger utility power grid.

Alabama Power's Smart Neighborhood consists of 62 homes in Hoover, Alabama. Each home is equipped with enhanced energy-efficient home technologies. Photo courtesy: Southern Company

The microgrid includes 11 rows of solar panels with more than 1,200 modules that convert light from the sun into energy. Solar panels can supply power to both the neighborhood and existing electric grid. Photo courtesy: Southern Company

City of Oak Ridge partners

on advanced urban planning tool

by Ashley Huff
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ORNL's Urban Dynamics Institute is working with the city of Oak Ridge to develop a sensor network and web tool that will evaluate trends in urban activity and help cities plan their development more effectively.

The technology, called UrbanSense, shows how a community is being used, not just where people live and work, say UDI researchers Teja Kuruganti and Gautam Thakur from ORNL's Computer Science and Engineering Division.

"We are using sensors to generate observations and insights to help cities measure their growth and success," Kuruganti said. "We want to give cities like Oak Ridge a better sense of their population distribution and dynamics."

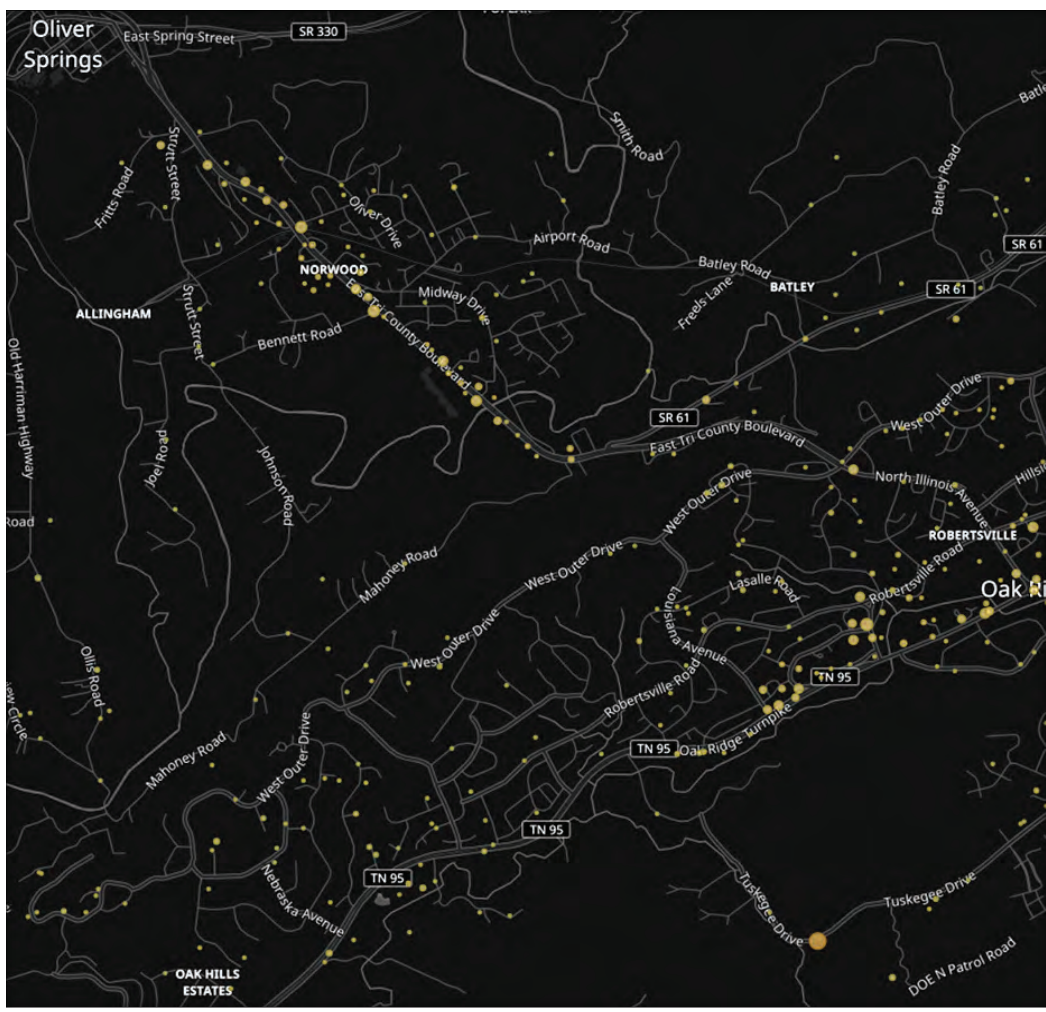
Kuruganti and Thakur are collaborating with Oak Ridge's director of administrative services, Bruce Applegate, on the design and deployment of the system.

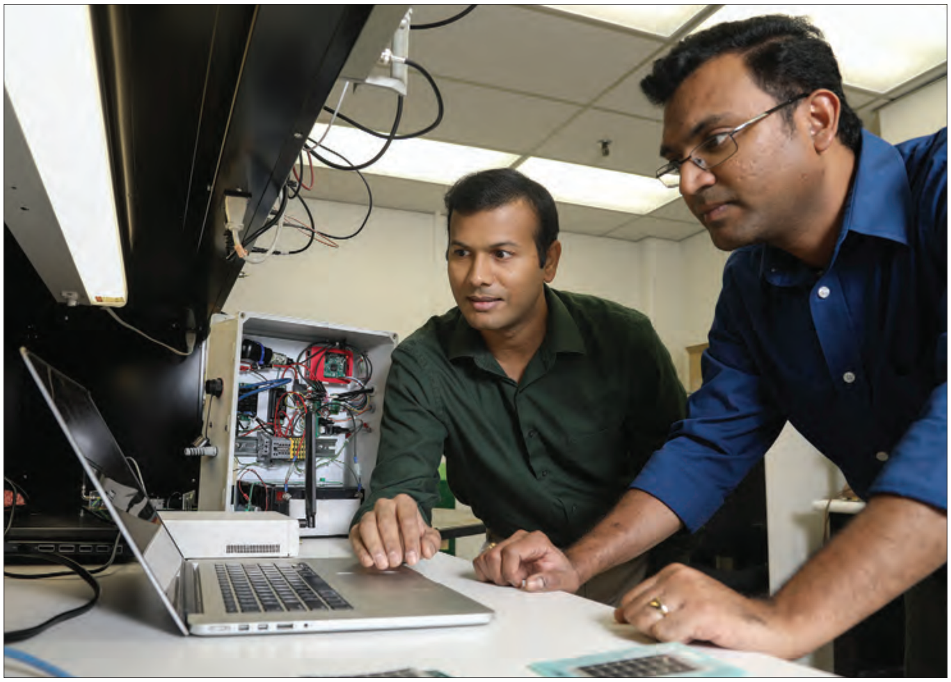
UrbanSense integrates information from virtual and physical sensors to give a bird's-eye view of activity. The cloud-based system, supported by ORNL servers, captures trends and displays the information via an online dashboard.

The system reports real-time population dynamics using anonymous data passively collected from open-source or volunteered information. For instance, to help estimate population density, UrbanSense uses open broadcasts made by cellular towers as mobile networks plan for customer capacity; it doesn't pick up information about individual phones. Other data sources include online public data sets such as AirNow.gov and self-reported data from social media, such as Facebook "check-ins" or Twitter posts.

Once installed, commercially available physical sensors that monitor traffic flow and water and air quality will provide Oak Ridge with additional information relevant to citywide strategic planning. "The longer they are in place and the more data they collect, the better the city's sense of its trends will be," Thakur said.

UrbanSense passively collects anonymous, open-source data from cellular towers and other sources to generate real-time estimates of population density in cities. Insights on how people interact with urban infrastructure help cities like Oak Ridge, Tennessee (below), assess their needs and plan effectively for future development. Image credit: Gautam Thakur, ORNL





Gautam Thakur, left, and Teja Kuruganti demonstrate UrbanSense, a novel sensor network aimed at helping cities manage their growth and evaluate future development opportunities. Image credit: Jason Richards, ORNL

U.S. cities typically rely on static data, gathering population insights from census reports and other sources of infrequently updated information. These data are limited to "ambient" populations, or activity averaged over 24 hours. They may provide information on where people live and work, but they do not tell cities where people are at a given time of day.

To know how many people travel in and out of a city, which events are attended and which roads are used most frequently—the kinds of questions relevant to city-level planning—minute-by-minute population data is essential.

"UrbanSense augments existing technologies by offering near-real-time estimates of urban population activity," Thakur said. "This is a huge improvement over anything cities have had before."

Cities can use this fine-resolution population and traffic data to optimize infrastructure, evaluate retail markets, manage traffic for local events and more strategically assess their development potential.

"For Oak Ridge, the UrbanSense platform has provided a 21st-century tool to analyze the rapid changes our community is undergoing through both commercial and residential development," Applegate said. "The real-time data collected will not only increase our understanding of the city's usage by residents and visitors but will also aid in the selection and prioritization of city-funded projects."

In adopting the prototype, Oak Ridge is poised "to demonstrate the ways UrbanSense can shift a municipality from a day-to-day approach to a longer-range vision of urban development," Applegate said.

By design, UrbanSense is scalable with additional sensors, so it can be tailored to the unique needs of individual cities and the full range of trends they want to examine.

The next step is to expand on the prototype. "We want to bring the technology to other cities," Kuruganti said.

SOLVING BIG PROBLEMS WITH ARTIFICIAL INTELLIGENCE

The Problem

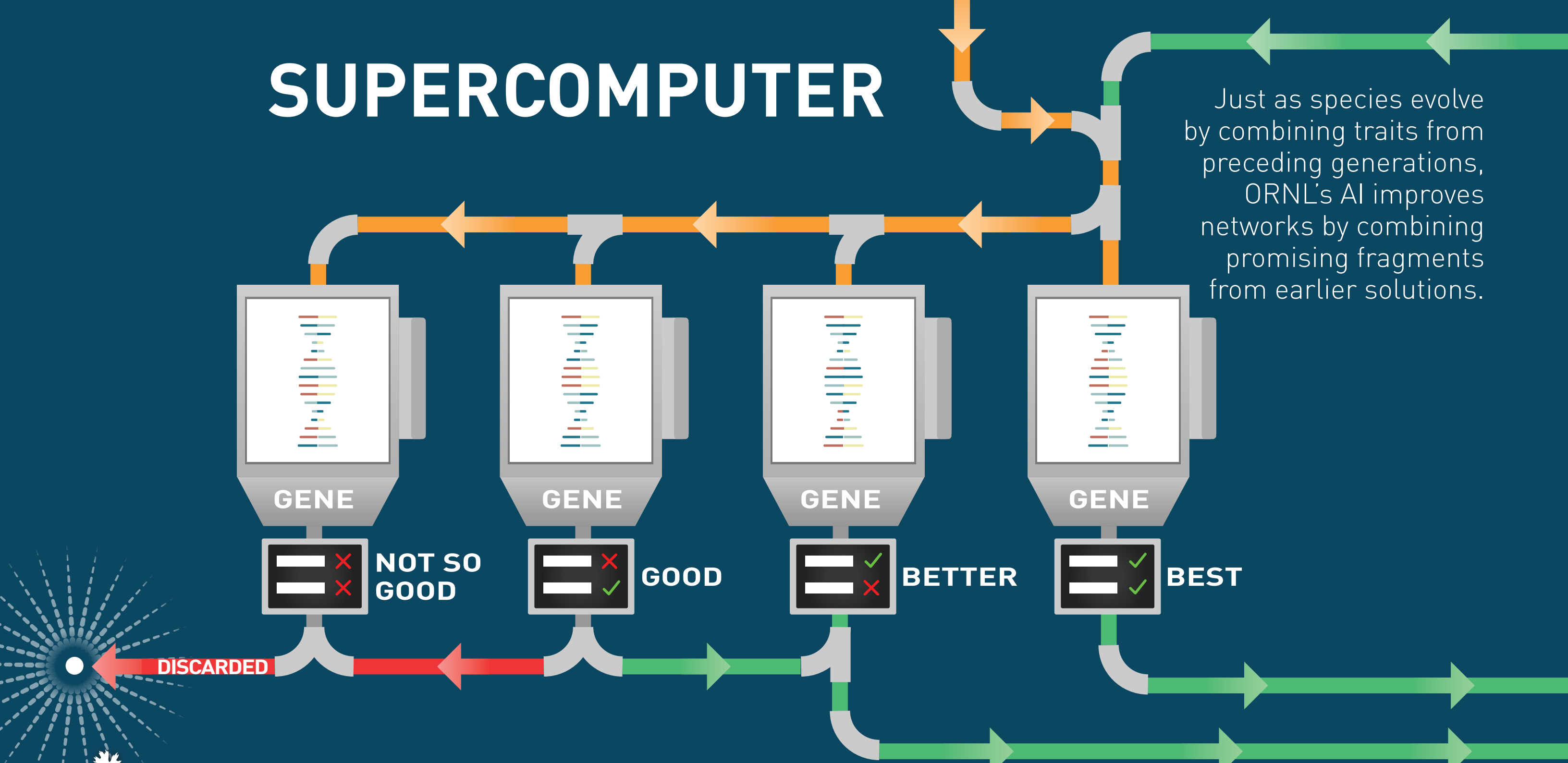
Bill is an instrument scientist at ORNL's Spallation Neutron Source. Researchers generating enormous numbers of datasets at SNS often ask Bill how they should interpret the information.

There are many possibilities, and finding the best can take hours, days, even weeks. Artificial intelligence (AI) provides a faster, more efficient way to help researchers identify a solution.

The Process

Bill turns to the lab's Computational Data Analytics Group, which uses supercomputers such as ORNL's Titan and Summit to rapidly produce and test thousands of complex deep-learning networks, saving researchers the months it would likely take to develop their own.

The group's deep-learning tools evaluate, evolve, and optimize neural networks (i.e., AI networks modeled after the human brain) for large scientific datasets. They test and train thousands for each science problem and quickly identify the one best suited to the task at hand. This process is iterative, with the best performers merged in various ways, allowing them to evolve into even better matches.



Just as species evolve by combining traits from preceding generations, ORNL's AI improves networks by combining promising fragments from earlier solutions.

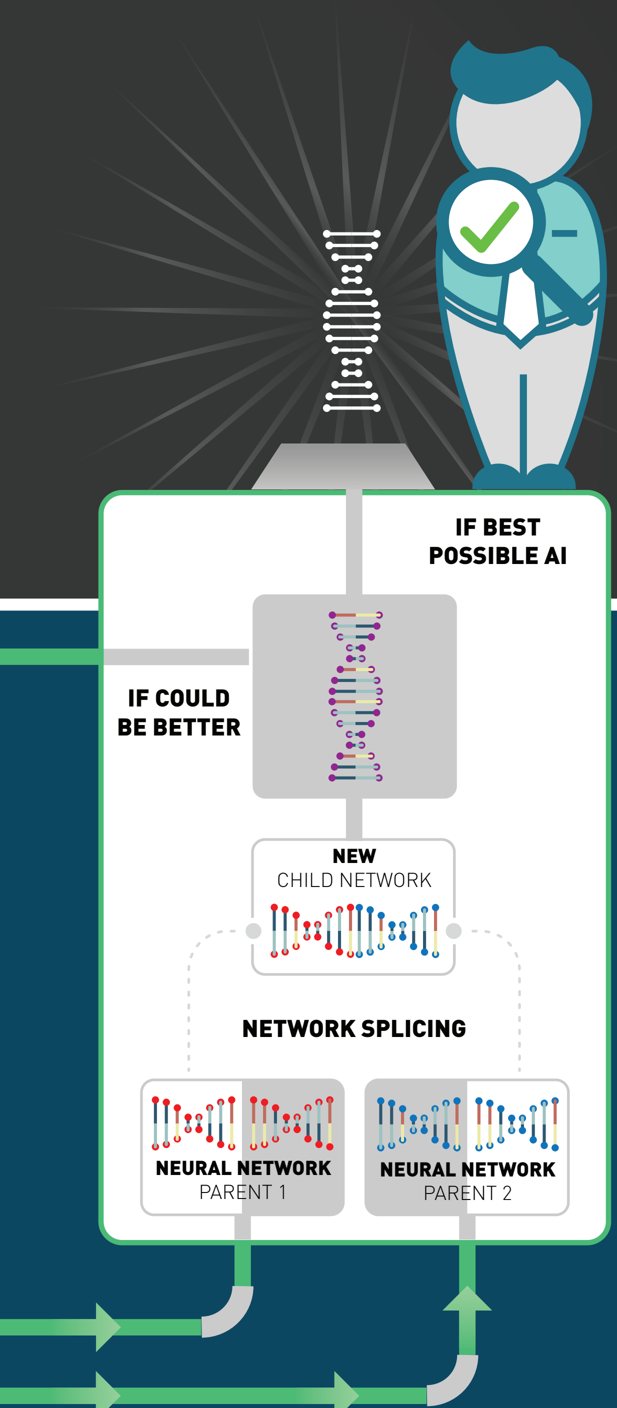
The Solution

The best-performing network does not require a supercomputer; researchers can use their personal computing systems to rapidly and efficiently analyze massive experimental datasets and, by extension, achieve breakthroughs faster. This "hub-and-spoke" model (the best network can be used with other, similar datasets) allows different types of researchers to reap the benefits of the lab's AI expertise and world-class computing power.

Applications

AI is helping scientists to:

- Analyze images of atomic trajectories during reactions, allowing for an enhanced understanding of the laws governing materials
- Decipher the interaction of neutrinos with ordinary matter
- Process the many data sources necessary to create robust cybersecurity
- Understand complex ecosystems, allowing researchers to decipher the differences in species for ecosystem optimization
- Analyze decades of health data, paving the way for new treatments



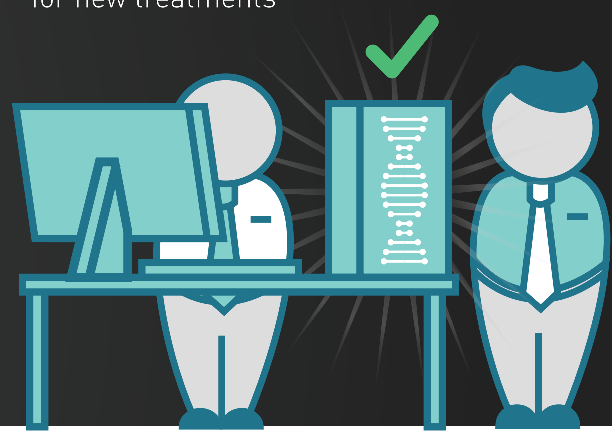
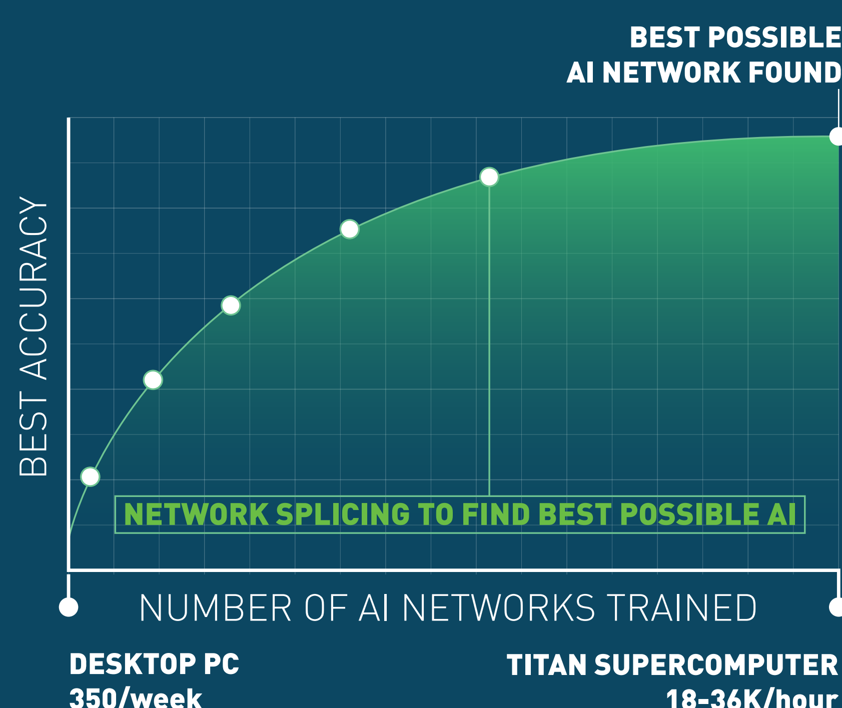


Image credit: Adam Malin, ORNL



Better catalysts

boost yields, decrease costs

by Dawn Levy
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For some crystalline catalysts, what you see on the surface is not always what you get in the bulk, according to two ORNL-led studies.

Investigators discovered that treating a complex oxide crystal with either heat or chemicals caused different atoms to segregate on the surface. Such surface reconstruction created catalysts with different behaviors, which encouraged different reaction pathways and ultimately yielded distinct products.

By using thermal and chemical treatments, catalyst designers may be able to drive industrially important chemical reactions to improve yields of desired products and reduce unwanted products so that post-reaction separation costs can be significantly lowered.

"The surface of a catalyst is a playground for the molecules to do the chemical reaction," said ORNL chemist Zili Wu, the senior author of two recent papers about the effect of the atomic composition of a catalyst surface on acid–base chemistry. "If you can tune your catalyst to obtain the desired product—i.e., achieve high selectivity—you will reduce the side products. Then you don't need costly and energy-intensive downstream chemical separations."

The researchers surveyed four catalysts of perovskite with atomic composition ABO3, where A is a rare-earth metal cation (i.e., positively charged ion), B is a transition-metal cation and O is oxygen.

Treating a perovskite with heat resulted in a catalyst with more A atoms on its surface, whereas treating the same perovskite with chemicals produced more B atoms on the surface.

The experiments showed that the catalyst could be tuned with different treatments.

"If you have a basic surface, an AOx-dominated surface, it will do the base–catalyzed reaction to acetone," Wu said. "If you have an acid surface, a BOx-dominated surface, it adapts to that route, to propylene. The same perovskite subjected to different treatments could produce a desired product, such as acetone or propylene, in yields ranging from 25 to 90 percent."

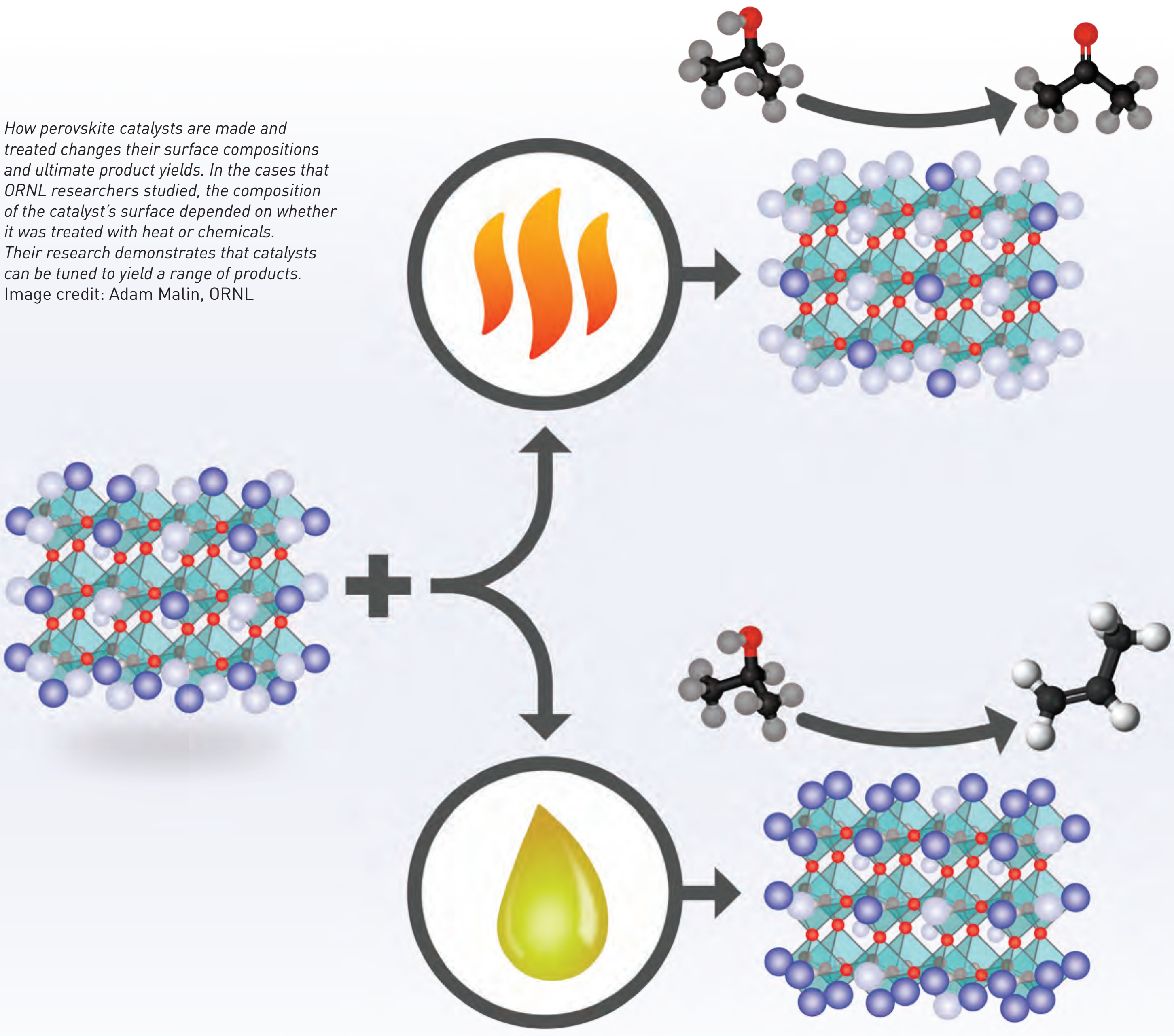
> *"The geometry and the composition of the [positively and negatively charged ions] are arranged differently when you have different facets. That can give you quite different chemical reactivity."*
>
> — ORNL chemist **Zili Wu**

The scientists were the first to systemically study how different perovskite surface compositions affect acid–base catalysis. The knowledge gained could provide a route to selective conversion of biomass into desired chemicals.

To test the acid–base performance of the treated perovskite catalysts, the researchers studied a model reaction, the conversion of isopropanol—basically, rubbing alcohol. Depending on the pretreatment conditions, the perovskite could selectively turn the alcohol into propylene (a building block of plastics) through a dehydration reaction, or acetone (an industrial solvent) through a dehydrogenation reaction.

The scientists used X-ray diffraction to characterize the bulk of a catalyst and numerous techniques to characterize its surface. To learn if element A or B predominated on the perovskite surface, they employed scanning transmission electron microscopy, adsorption microcalorimetry and infrared spectroscopy to examine catalyst nanoparticles.

Low-energy ion scattering performed at Lehigh University shot an ion at a nanoparticle, and the energy lost when the ion bounced back revealed compositional details of the very top surface



How perovskite catalysts are made and treated changes their surface compositions and ultimate product yields. In the cases that ORNL researchers studied, the composition of the catalyst's surface depended on whether it was treated with heat or chemicals. Their research demonstrates that catalysts can be tuned to yield a range of products. Image credit: Adam Malin, ORNL

layer. Lessons learned about surface composition from all these experiments aided computations to predict reaction pathways. Catalytic measurements confirmed the impact of surface segregation on the acid–base catalytic properties of the perovskite material.

In the future, the researchers will explore reconstruction processes of perovskite catalyst surfaces with different crystallographic planes.

"The geometry and the composition of the [positively and negatively charged ions] are arranged differently when you have different facets," Wu explained. "That can give you quite different chemical reactivity."

The researchers are currently expanding their work to tune the surface planes of perovskites to understand and optimize oxidation and reduction reactions beyond acid–base ones, which could be used in the conversion of shale gas (mostly methane) to valuable chemicals.

For more information:
go.usa.gov/xn7aU

Hydropower's future is small & modular

by Stephanie Seay
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Harnessing the power of water is a practice that has been around for thousands of years, from the ancient Greeks' use of waterwheels to grind wheat to today's massive hydroelectric dams that supply power to millions of customers.

But given the high price tag, potential environmental impact and difficulty of licensing large dams, the future of hydropower may shift to standardized projects with a smaller footprint, built with less customization and lower cost on a variety of waterways.

That's the future envisioned by Standard Modular Hydropower, a project at ORNL designed to accomplish much of the legwork for hydropower developers by identifying potential sites and helping inventors design affordable, functional systems that can be installed on smaller rivers and streams.

"There is a lot of potential for new hydropower development in the United States," said Adam Witt, a hydropower systems research engineer who leads the SMH project. "But it's very challenging to build that potential out, mainly because we haven't figured out how to reduce environmental impacts, the cost is really high, and the timeframe to get through the regulatory process is very long."

As a result, most of the new hydropower added in the past 20 years has been from upgrades to existing facilities or electrification of nonpowered dams. The goal of the SMH project is to kindle a renaissance of new hydropower, which now accounts for 6.5 percent of total electricity generation, making it the largest source of renewable energy in the country.

> *"We want to get people to design things that are useful in a lot of different areas and not just specific to one site. That way the design and development cost drops, you can produce things more cheaply and meet the needs of more clients."*
>
> — ORNL senior scientist **Mark Bevelhimer**

Adam Witt, left, and Mark Bevelhimer are using data on the nation's waterways to encourage small, modular hydropower project development. Image credit: Jason Richards, ORNL

The ideal SMH design would harness power from the natural flow of a river and have a capacity in the hundreds of kilowatts up to 10 megawatts, with power supplied to a local utility system or transmitted directly to a nearby end user. Developers could be independent power producers, investor-owned utilities, electric cooperatives or municipalities.

SMH technology would be fully submerged in waterways, eliminating the need for a separate, large powerhouse for generators. The result would be unlike anything seen in conventional dam designs. Witt and his collaborators are hoping that by providing detailed information on waterways across the country, they will encourage inventors to create hydropower projects that are multipurpose, generating electricity while improving the health of the watershed.

The SMH project at ORNL is developing a site classification tool to sort stream segments into groups with similar characteristics—everything from water flow rates to the type of bedrock and sediment, from water quality and power potential to fish species and recreational usage. The publicly available, interactive database will include a mapping tool and provide hydropower entrepreneurs and developers a list of locations where their hydropower designs can best be applied.

"We want to get people to design things that are useful in a lot of different areas and not just specific to one site," said ORNL's Mark Bevelhimer, a senior scientist who has been heading data collection and analysis for the site classification effort. "That way the design and development cost drops, and you can produce things more cheaply and meet the needs of more clients."

Developers may search for a variety of characteristics, Bevelhimer noted. They may want to avoid waterways with migratory fish species so they don't have to add fish ladders. Or they may seek out sites with poor water quality if their design provides the added benefit of aerating rivers with low levels of dissolved oxygen.

A holistic understanding of river physics, ecological interactions, river resource use by humans and the regulatory process puts SMH in an excellent position to encourage future hydropower development, Bevelhimer added.

ORNL's interdisciplinary environment has been essential to developing the SMH project, Witt said, by bringing together experts in hydropower engineering, aquatic ecology and computational science to think about ways to jump-start small hydropower development.

"The big challenge is to solve little pieces of the problem to get to a better overall solution," Witt said. "In the end, those little pieces have the potential to add up to transformative change."

Cell's 'vacuum cleaners' modeled atom by atom

by Jonathan Hines
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In the fight against cancer, cancer cells often find ways to fight back. One means is by stocking the cell membrane with proteins that pump foreign substances—including anticancer drugs—out of the cell. This trait can result in multidrug resistance that undermines the effectiveness of cancer treatment.

To combat this defense mechanism, scientists are turning to supercomputers and molecular dynamics to better understand the function of a membrane transport protein called P-glycoprotein, or Pgp. In healthy cells, Pgp acts as the cell's vacuum cleaner, removing unwanted or toxic substances. But to treat cancer, doctors sometimes need to temporarily pull the plug on these molecular pumps. The task requires developing targeted drugs based on a thorough understanding of Pgp's makeup and mechanics.

Using ORNL's Titan supercomputer, a team led by computational biophysicist Emad Tajkhorshid from the University of Illinois at Urbana-Champaign uncovered new details that could help this endeavor, producing the first experimentally verified atom-by-atom look at a mammalian Pgp in its outward-facing state (open to the outside of the cell).

"These findings could aid in drug discovery, where researchers are looking for better Pgp inhibitors—drugs that block transporter function and make it easier for anticancer drugs to do their job," said Sundarapandian Thangapandian, a team member and postdoctoral researcher at UIUC.

To gain a more comprehensive picture of the protein, Tajkhorshid's team relied on detailed molecular measurements captured by a Vanderbilt University team using a spectroscopy method called double electron–electron resonance. These experiments provided precise information that allowed the team to construct a model based on data from a mammalian Pgp both in its inward-facing state (open to the inside of the cell) and in its outward-facing state.

With the newly minted model, Tajkhorshid's team, in effect, possessed a lock in need of a key. That key came in the form of Titan. Using the molecular dynamics code NAMD, the UIUC team explored Pgp's mechanics by dividing the protein into five distinct simulation sets. The setup allowed the team to scrutinize Pgp's components in isolation on Titan before bringing them all together. Thangapandian, who managed the simulations, compiled 300 nanoseconds of simulation time for each subunit—aggregating 1.5 microseconds of the Pgp model in total.

The substantial sum of simulation data unlocked a trove of new insights, including how Pgp uses adenosine triphosphate, or ATP, the universal energy currency of the cell, to close and open. The team found the mechanism consists of a "two-stroke" sequence.

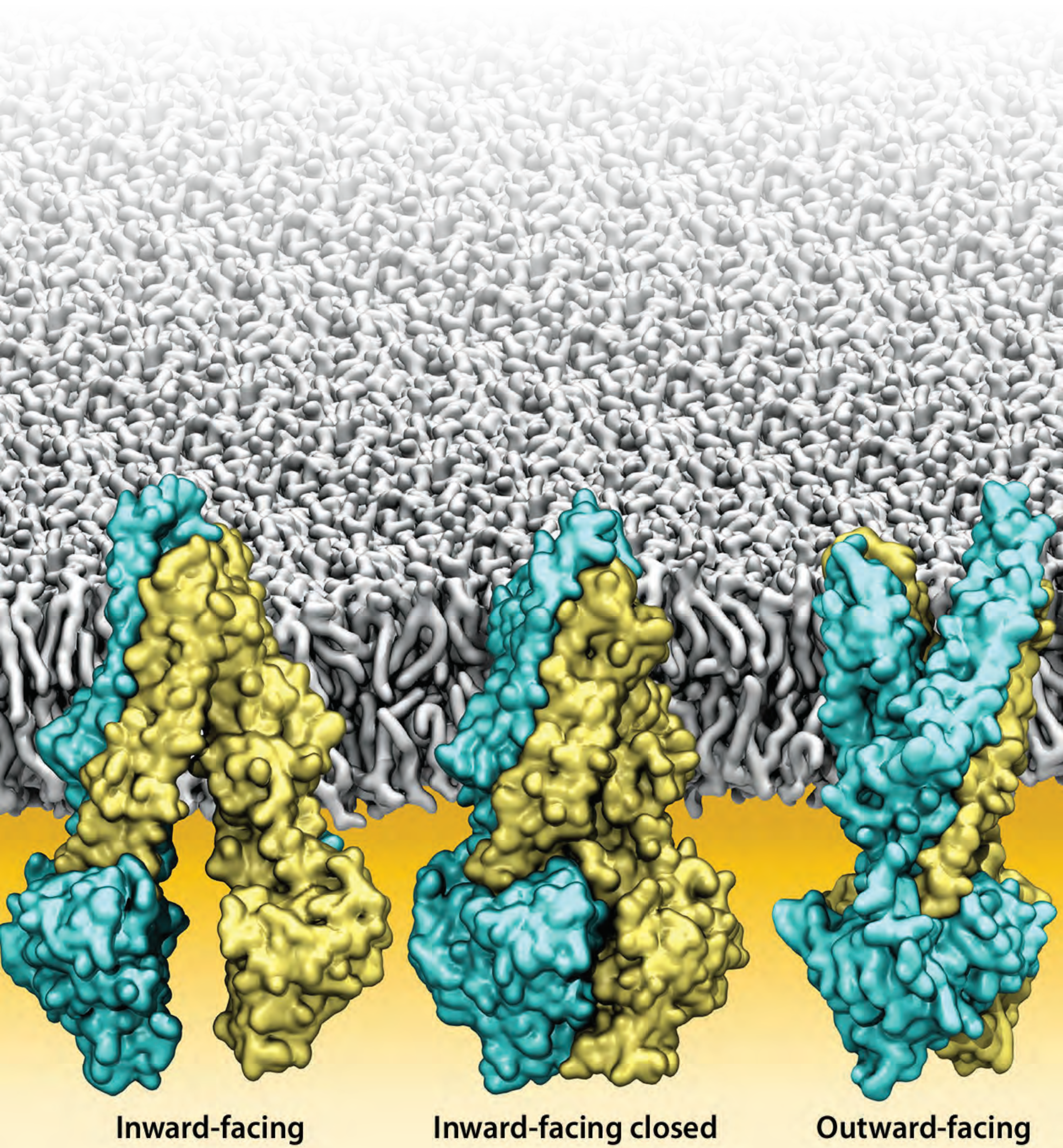
"This means one ATP is needed to close the inner side of the protein, and a second is needed to open the outer side," Thangapandian said.

In the midst of this energy transfer, the team documented 60 interactions involving different atoms. The new mechanics play an important role in bringing together Pgp's nucleotide-binding domains (the docking site for ATP) into a single chemical structure, a process known as dimerization. Additionally, the team discovered factors that contribute to Pgp's structural stability in its outward-facing state. The findings include a "salt bridge"—an ionic coupling between positively and negatively charged amino acids—and interactions between the protein and adjoining lipids in the cell membrane that contribute to the protein's structural integrity.

With Pgp's two end states now well characterized, Tajkhorshid's team is shifting its attention to the action in between, work that could lend additional insights to biologists and medicinal chemists.

"We want to give researchers focused on Pgp a set of stable intermediate states to target as well," Thangapandian said. "That would really improve the effectiveness of the drug discovery process."

The membrane transport protein P-glycoprotein transitioning from its inward-facing state to its outward-facing state. Image credit: University of Illinois at Urbana-Champaign


Inward-facing
Inward-facing closed
Outward-facing

Critical neurotransmitter

modeled on Titan

by Katie Jones
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The chemical neurotransmitter dopamine is critical to sending and receiving signals in the nervous system linked to motor movements, learning, and habit formation. No wonder many therapies for drug addiction and diseases related to the aging brain, such as Parkinson's disease, target dopamine uptake.

Clustered in regions of the midbrain near the spinal cord is the dopamine transporter, or DAT, a large protein with many molecular components that pumps dopamine across the membrane. To develop drug therapies for addiction and disease, researchers need to understand how to lock and unlock DAT.

Unfortunately, there is no single key. Stimulant drugs like amphetamines can induce DAT into structures that flex open the protein to the outside environment and "flood" neurons with dopamine, whereas Parkinson's results from the degeneration of dopamine-rich areas of the brain and, often, the inhibition of DAT.

Using the nation's most powerful supercomputer, ORNL's Titan, a team from Weill Cornell Medical College of Cornell University led by Harel Weinstein modeled the complex cascade of molecular interactions that activate DAT.

One stimulus that helps unlock DAT is sodium. Positively charged sodium ions are abundant outside the cell and can bind to and change the shape of DAT, ultimately enabling dopamine to enter the cell. With simulation data from Titan, Weinstein's team developed a kinetic model that describes how molecular motions that reshape the DAT molecule cause a sodium ion to move from one end of the molecule to another, leading to dopamine uptake into the cell.

"When the DAT is fully loaded with two sodium ions and dopamine, its molecular shape undergoes dynamic changes, and one sodium ion from a binding site we call Na2 moves into the cell," Weinstein said. "This triggers the entire cycle. The transporter opens inward, releases dopamine and the other sodium into the cell, then turns around and repeats this cycle by capturing another set of dopamine and sodium ions."

The team wanted to capture the pathway of the sodium ion as it moved away from its binding site to be transported into the cell—a pathway that could reveal molecular interactions important to DAT function and, therefore, disease-related mutations.

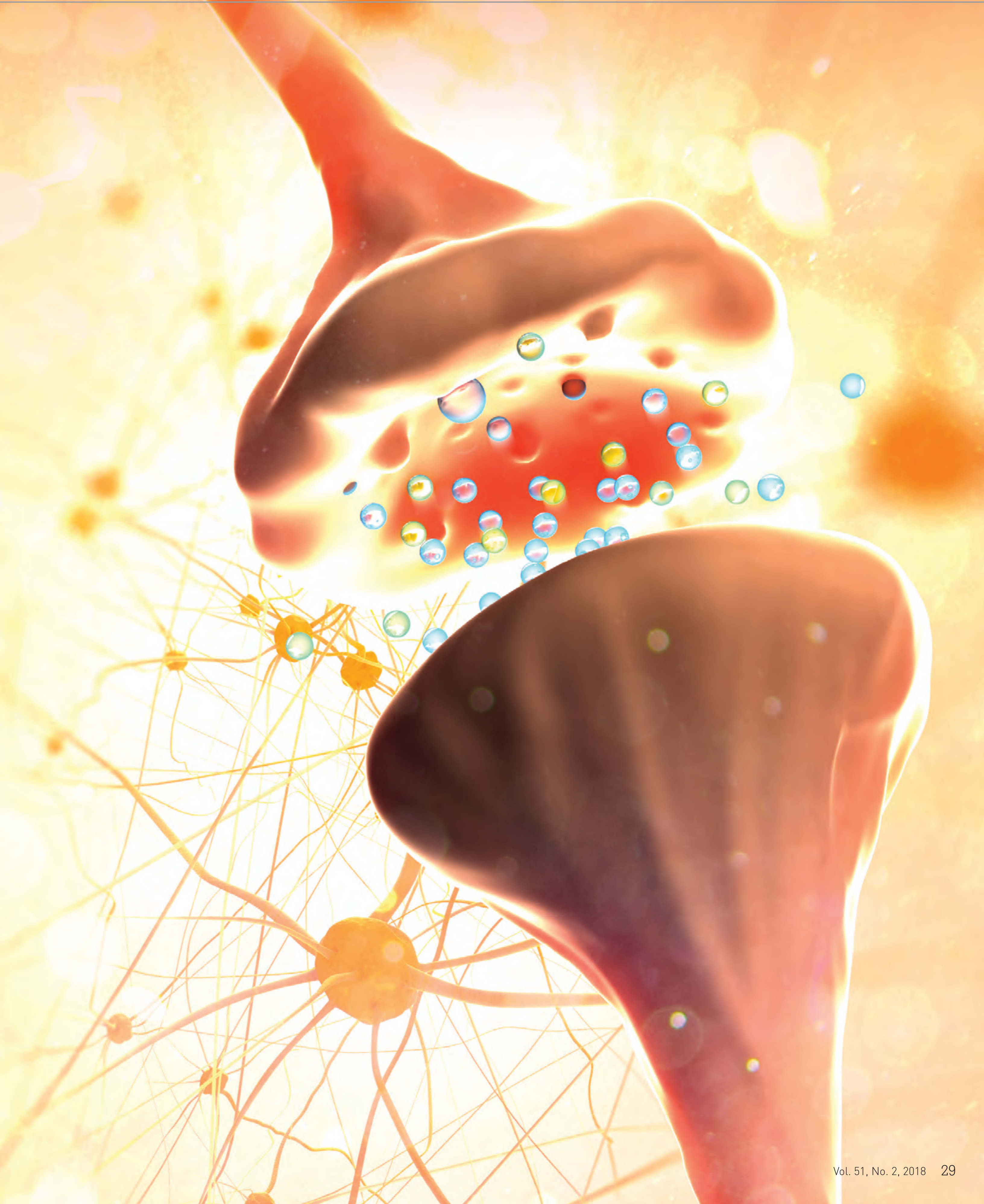
However, the movement of the sodium ion is hard to capture from experimental data and simple computational modeling. Using Titan, Weinstein's team set out to model the entire conformational space, or the space defined by all the possible DAT molecular interactions with the sodium ion.

First, the team modeled 50 separate, microsecond-scale molecular dynamics simulations of DAT embedded in a membrane model of the cell boundary surrounded by water, which amounted to about 150,000 atoms each. Based on the simulations, the team discovered water's role in penetrating the DAT molecule and helping move the sodium into the cell, creating several potential sodium pathways in the process.

Next, the team developed a kinetic model (known as a Markov State Model) of the sodium pathways by combining advanced data reduction and analysis techniques. Then they identified the most likely pathways based on which ones demonstrated the highest flux, or pumping rate across the neuron membrane. The model revealed three main pathways the sodium ion takes from its binding site. Each of these paths reveals a previously unknown relationship between the structure of the transporter and the way it accomplishes its tasks.

This new and comprehensive information can help scientists better understand dopamine uptake and neuronal signaling in the brain under normal and disease conditions and reveal new ways to regulate signaling and repair damaged neurons.

Whereas much of the interest in dopamine research is driven by the medical community, Weinstein said there are other applications of the sodium release model that extend beyond human biology, adding, "Because the transport of substances across membrane barriers is very important to biotechnology and energy-source developments as well, the new findings reveal essential details of an elemental process in those areas of research."



ORNL-developed alloy promises better fuel economy

by Jennifer Burke
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A new suite of aluminum-based alloys developed at ORNL could give automakers the key to achieving ambitious fuel economy goals. The aluminum-copper-manganese-zirconium alloys—or ACMZ—were developed in just under four years, lightning speed when it comes to developing a complex alloy.

Affordable, lightweight and capable of withstanding temperatures 100 degrees Celsius higher than commercially available automotive cast alloys, ACMZ is proving to be suitable for the next generation of internal combustion engines, enabling the industry to advance toward its target of 54.5 miles per gallon by 2025.

Current alloys inhibit engine efficiency because they soften at the peak temperatures present in highly efficient advanced engines. Automakers need an alloy that can take the heat, is durable and can be used in existing manufacturing processes. ACMZ meets all these parameters.

The journey to ACMZ began in 2012, with a challenge from DOE's Vehicle Technologies Office for a new high-performing alloy. A multidisciplinary team of materials, metallurgical and computational scientists led by ORNL's Amit Shyam stepped forward and embarked on the development plan with help from industry partners FCA US and Nemak U.S.A.

"We knew this was going to be a steep goal to achieve in four years," said Allen Haynes, leader of the Materials Processing and Joining Group at ORNL. "To put it in perspective, it typically takes 10 to 20 years to develop a new material."

Shyam's team first revisited history, comparing a group of industrially available aluminum alloys, including the RR350 alloy that evolved from a World War II aircraft application.

"One thing we do well at ORNL is apply scientific capabilities to solve challenging technological problems," Shyam said. "We have a unique combination of tools, expertise and capabilities that allow us to do interdisciplinary research beyond what industry can do. Our tools allow us to take a new approach to understanding an existing material.

"We started by looking at RR350. This alloy stood out from the rest because it had remarkable high-temperature properties but had poor casting behavior and wasn't affordable due to expensive nickel and cobalt additions," Shyam said.

The team put RR350 under the microscope and imaged and chemically analyzed it to the atomic scale, enabling a better grasp of its properties.

"We began to understand what happens to the structure and stability of the material as it goes through various temperatures and stresses and, in the process, discovered how to make it stronger and more castable while also eliminating expensive elements," Shyam explained.

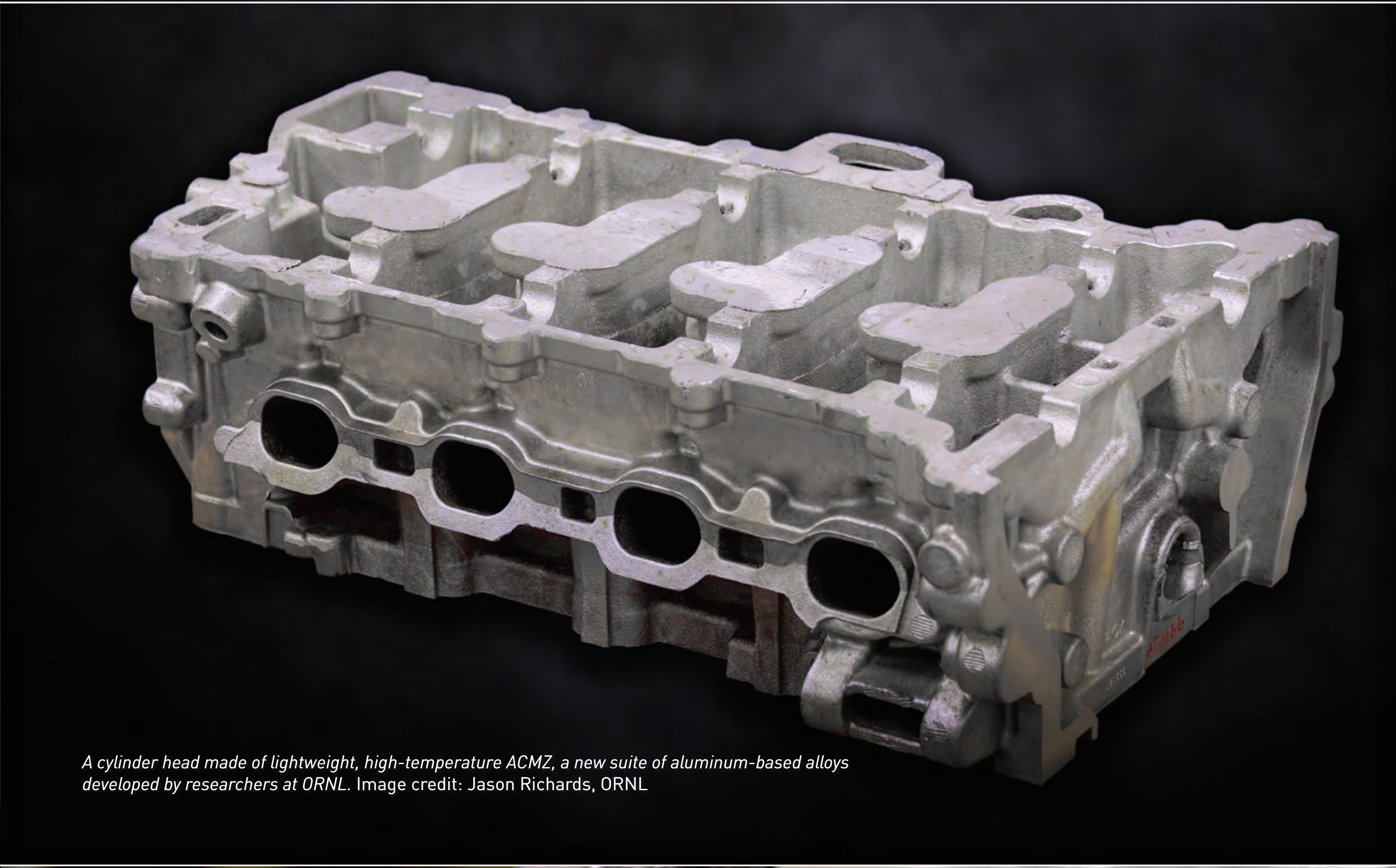
Using ORNL's Titan supercomputer, Shyam's team performed energy calculations on RR350 that provided key insight regarding its extraordinary stability.

With RR350 serving as the baseline, ACMZ was soon born.

"The combination of our experimental research, computational calculations and materials characterization capabilities, along with regular participation from our two industry partners, helped us develop ACMZ," Haynes said. "Early-stage research provided a fundamental breakthrough in metallurgy that was leveraged into the design of this new family of alloys."

Testing continues with FCA and Nemak to evaluate the alloy's durability in engine applications. A cylinder head cast from ACMZ successfully completed FCA's rigorous dynamometer test on a turbocharged engine in December 2017, and internal evaluations of ACMZ will continue throughout 2018.

"Everyone in the industry wants an alloy that has this combination of capabilities—easy to manufacture, able to be cast in complex designs, can take the heat and yet still offers required strength and endurance," Haynes said. "The potential for this new family of alloys to impact the automotive industry by expanding engine design space to enable affordable advances in fuel economy and performance is remarkable."



A cylinder head made of lightweight, high-temperature ACMZ, a new suite of aluminum-based alloys developed by researchers at ORNL. Image credit: Jason Richards, ORNL

The ACMZ alloys can be dropped into existing cylinder head manufacturing systems, such as industry partner Nemak U.S.A.'s casting process. Image credit: Nemak U.S.A.

Custom-designed alloy enhances nuclear safety

by Leo Williams
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The fuel rods at civilian nuclear power plants have been sheathed with an evolving zirconium alloy for the past six decades.

Zirconium was chosen as the preferred base metal in the 1950s by Hyman Rickover, then a U.S. Navy captain who would rise to admiral as he led the successful effort to use nuclear power for ships and submarines. The alloy and the light-water reactors in the nuclear navy were adapted by the nuclear power industry and today dominate plants throughout the world.

Zirconium absorbs very few of the neutrons that drive a nuclear reactor, so zirconium alloys made sense as a fuel cladding—as long as the reactor operated as planned. When things go wrong and a reactor loses its cooling water, however, the zirconium can make a bad problem worse.

In response, DOE's Office of Nuclear Energy enlisted an ORNL-led team to develop a fuel cladding that gets the job done without zirconium. The new material, an alloy of iron, chromium and aluminum, should give plant operators substantially more time to react in an incident such as a station blackout.

"The issue is you have anywhere between 20 and 40 tons of zirconium metal in these reactor cores," explained ORNL nuclear engineer Kurt Terrani, who heads the project. "Zirconium reacts with steam at high temperature, and when it reacts it produces a lot of heat and a lot of hydrogen."

The job for Terrani's team, part of a consortium led by General Electric, was to create a zirconium-free alloy that would generate as little hydrogen as possible during an incident while at the same time matching the performance of the nuclear fuel rod cladding that is in use today.

The project was out of the ordinary for at least three reasons, Terrani explained.

In the first place, the team was not interested in testing existing alloys to see if one might be appropriate. Instead, it designed the new alloy from scratch with a diverse team that included experts in nuclear engineering, materials science, radiation effects, corrosion, thermomechanics and alloy fabrication.

The approach made use of the wide range of tools and expertise available at ORNL, DOE's biggest science and energy laboratory. The new cladding also underwent testing at ORNL's High Flux Isotope Reactor and Idaho National Laboratory's Advanced Test Reactor, as well as the Halden research reactor in Norway.

"This was by no means an Edisonian approach," Terrani said, alluding to the trial-and-error approach made famous by Thomas Edison's search for a light bulb filament. "We worked with knowledge and tools that were not available in Rickover's day. We designed an alloy that we knew was going to work. I'm not surprised that this alloy behaves so well under different conditions; we designed it to do so."

Secondly, the team was able to identify and produce the alloy in six years, which is extremely fast in the nuclear industry. Conventional wisdom says the project should have taken twice the time, Terrani said.

Thirdly, he added, the project is unusual because it is not ongoing.

"The other thing I'm very proud of is we are ready to stop working on this," he said. "We feel like we delivered it, the industry is running with it. We want to put a big fat red bow on it."

The new cladding was placed in a reactor at Southern Nuclear's Hatch Nuclear Power Plant in Georgia for testing in February, Terrani said, and subsequent installations are planned.

The iron-chromium-aluminum fuel cladding alloy designed by an ORNL-led team will give nuclear plant operators more time to react in case of an incident. Image credit: Jason Richards, ORNL

Neutrons search for clues to combat bacterial threats

by Elizabeth Rosenthal
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The discovery of penicillin almost 90 years ago ushered in the age of modern antibiotics, but the growth of antibiotic resistance means bacterial infections like pneumonia and tuberculosis are becoming more difficult to treat.

Researchers at ORNL's Spallation Neutron Source are working to make sense of this phenomenon. Using the Macromolecular neutron diffractometer instrument at SNS, known as MaNDi, they hope to better understand how bacteria-containing enzymes called beta-lactamases resist the beta-lactam class of antibiotics—antibiotics containing a beta-lactam ring made up of organic compounds.

"We are looking for answers on a fundamental science level," said MaNDi instrument scientist Leighton Coates. "We have the machinery to explore these interactions using neutrons."

With neutrons, the team can observe firsthand—without damaging the biological samples—how beta-lactamases break down drug compounds.

Beta-lactam antibiotics interfere with penicillin-binding proteins, which are responsible for constructing bacterial cell walls. By disrupting this process, antibiotics destroy invading bacteria and fend off lethal infections.

In response, bacteria have evolved to counteract antibiotics by producing beta-lactamases. These enzymes serve as natural catalysts, breaking open the beta-lactam rings in antibiotics to deactivate their antibacterial properties.

Beta-lactam antibiotics are commonly prescribed because of their high specificity and low toxicity. However, as the number of antibiotics increases, so too does the number of resistant bacterial strains. Under these circumstances, even common respiratory tract and bloodstream infections can become dangerous.

Patients with existing health problems are more likely to contract bacterial infections and encounter resistant bacteria, but human behavior can also contribute to antibiotic resistance in healthy individuals, such as when people take unnecessary or expired drugs.

As the perils of bacterial resistance continue to manifest in the emergence of incurable "superbugs" and the reemergence of various infectious diseases once thought under control—if not eradicated—scientists are increasingly determined to investigate contributing factors.

"We are studying not only how these antibiotics break down but also how the bacteria are evolving to resist them," Coates said.

Such information could help medical professionals tackle one of the most significant and wide-reaching threats to public health in the world today. The Centers for Disease Control and Prevention estimates that antibiotic resistance affects about 2 million people every year in the United States alone.

Researchers are developing new drugs that rely on substances called inhibitors to block beta-lactamases, but these methods are not infallible.

Bacteria have fleeting lifespans that allow for rapid evolution. As a result, beta-lactamases can quickly adapt to resist new antibiotics. Medical researchers seek to stop, or at least slow, this constant cycle.

"When a new drug is introduced that the beta-lactamases can't break down, bacteria mutate and create new enzymes to attack the antibiotic," said Patricia Langan, a postdoctoral researcher at SNS. "It's a constant battle to stay ahead of them."

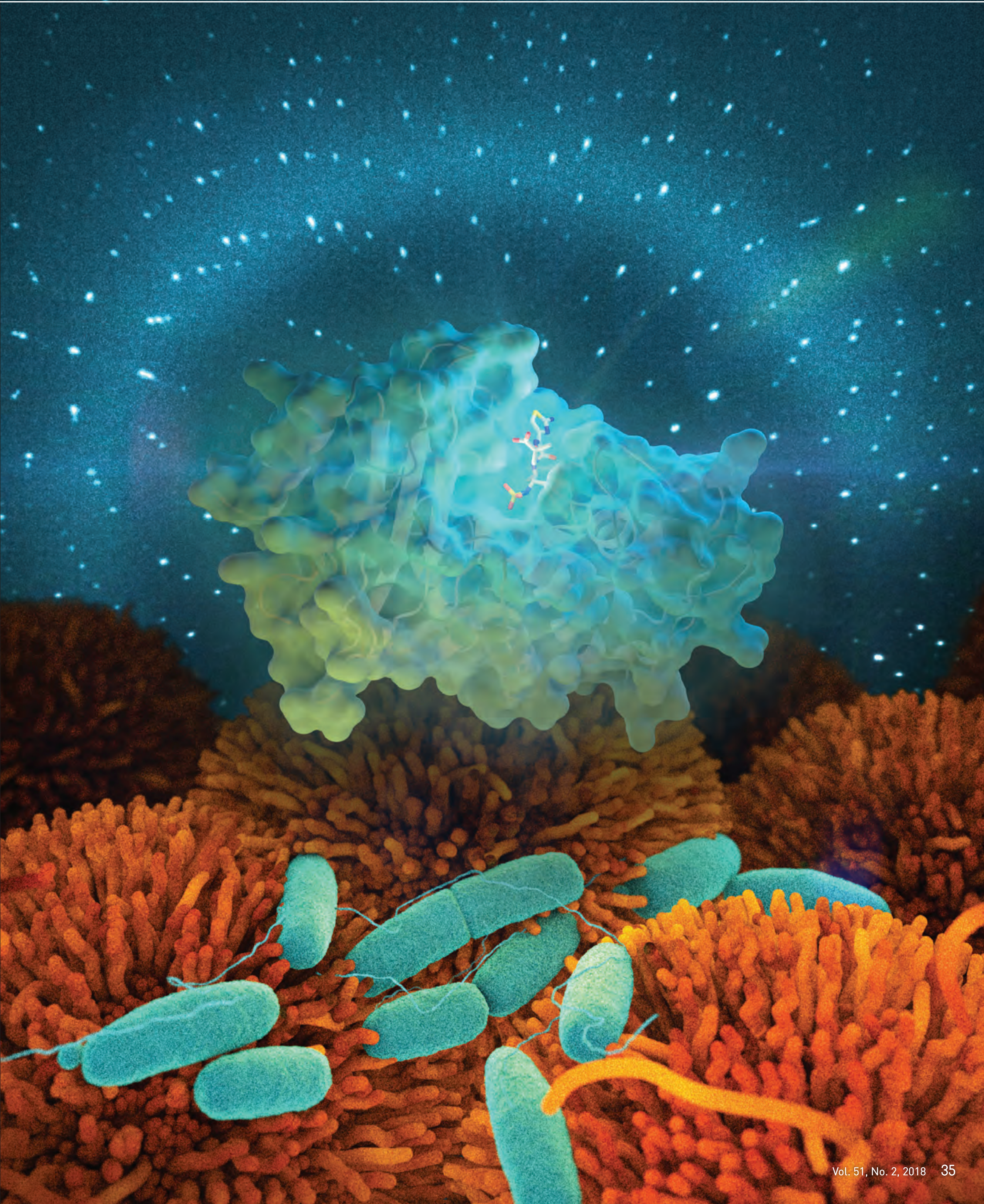
To date, the team has studied how beta-lactamases break down antibiotics like aztreonam, penicillin, and cefotaxime.

"We're going more in-depth into exactly what is happening on a chemical level, and hopefully our research will help with future inhibitor design and drug development," Langan said.

The team's most significant discovery from this work involves demystifying the catalytic mechanism in beta-lactamases. They studied key amino acids that help break down beta-lactam antibiotics and identified their roles in this biochemical reaction. By studying proton transfers within these amino acids, the researchers can uncover the inner workings of beta-lactamases.

"We're finding all sorts of nuances," Coates said. "By using neutrons, we can work out the protonation state of these important amino acids, and from there we can deduce what's going on in the catalytic mechanism."

Bacteria-containing enzymes called beta-lactamases (light blue mass above) break down antibiotics and allow bacterial infections to develop and spread through human cells (orange). Neutrons help explain how resistant bacteria (light blue rod shapes) are evolving to negate the effects of the beta-lactam class of antibiotics.
Image credit: Thomas Splettstoesser, SCIste



Neutrons probe ecofriendly enzyme

by Ashley Huff
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ORNL's Spallation Neutron Source has helped explain the workings of an ecofriendly treatment for water contaminated by chlorite, an industrial contaminant that's common world wide.

An international team led by the University of Vienna's Christian Obinger used neutron analysis, X-ray crystallography and other techniques to study the chlorite dismutase enzyme. This naturally occurring protein can break down chlorite, an industrial pollutant found in groundwater, drinking water and soils, into harmless by-products, but its catalytic process is not well understood. Understanding how the bacterial enzyme converts chlorite into chloride and oxygen may open possibilities for future applications in bioremediation and biotechnology.

Results published in *ACS Catalysis* also contribute to fundamental research on the enzyme's ability to produce oxygen. Oxygen generation is incredibly rare in nature and was once thought possible only by photosynthesis, so the enzymatic activity of chlorite dismutase has attracted interest from the scientific community beyond its environmental applications for clean water.

Exactly how chlorite dismutase works at a molecular level to break down chlorite has been debated since its discovery in 1996. The complexity of the enzyme's molecular structure and the difficulty of studying proteins with experimental methods present inherent challenges for researchers.

Like most enzymes, chlorite dismutase is a protein that catalyzes a highly specific reaction. The process is often environmentally dependent, meaning it works best within specific conditions, including temperature, concentration and pH ranges. Identifying the ideal conditions for the reaction is key to supporting bioengineering and large-scale production of chlorite dismutase to safely remove chlorite from the environment and potentially exploit the enzyme's oxygen generation.

Researchers isolated an unstudied Cyanothece strain of chlorite dismutase and examined the protein's crystal structure at specific pH values to determine the impact of pH on chlorite conversion.

Neutron analysis at ORNL's Spallation Neutron Source was especially helpful. The crystal's lack of symmetry required a particularly long data collection lasting several weeks on the facility's MaNDi diffractometer.

"This crystal is unusual in that it has very little symmetry, so an especially large number of reflections have to be recorded individually to get a complete data set," said Leighton Coates, MaNDi lead instrument scientist. "This would be a challenging and lengthy task anywhere, and it was only achievable in this time frame due to the large area detector coverage of the MaNDi instrument."

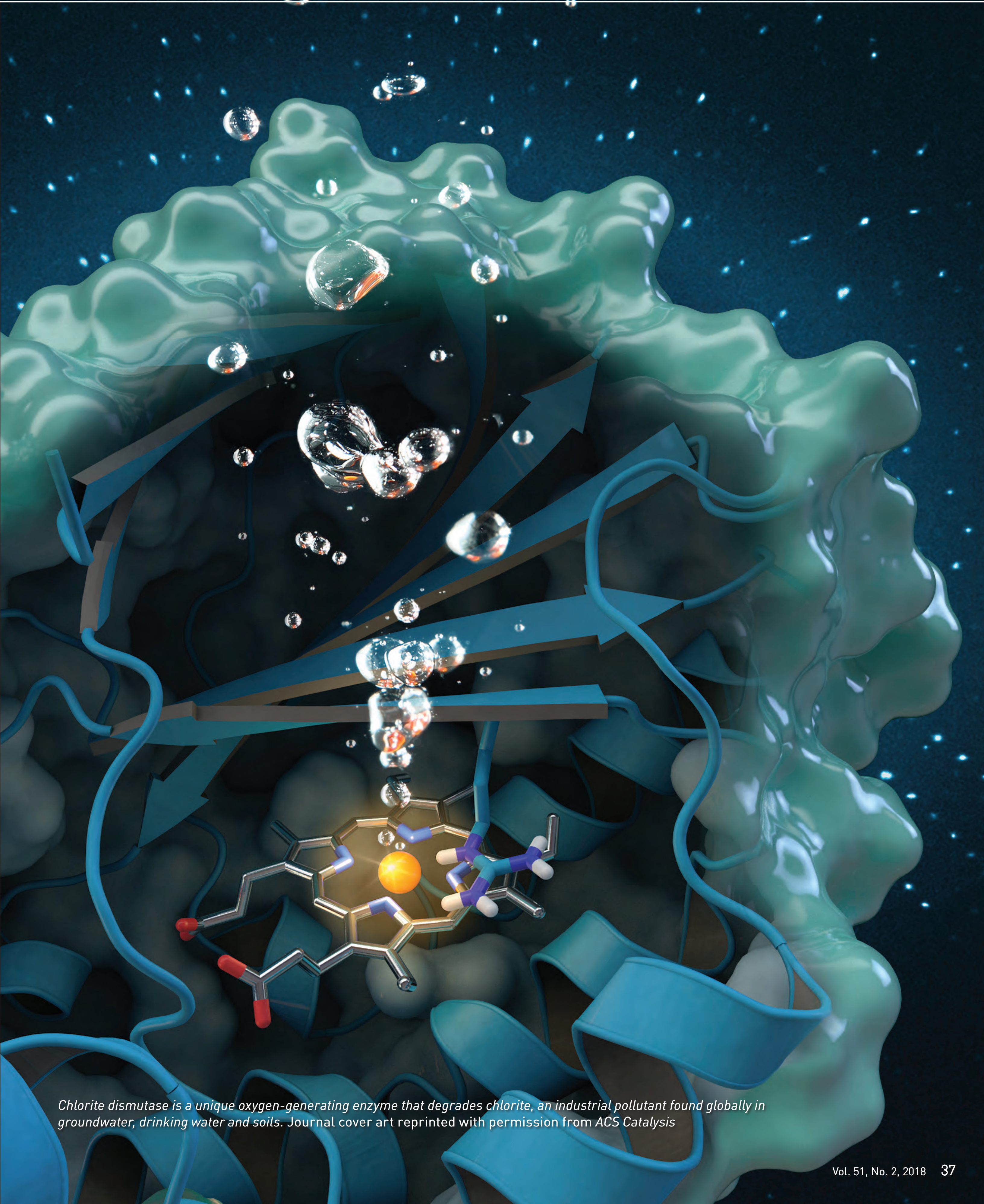
MaNDi enabled researchers to detect the protonation states of important amino acids thought to support the reaction. "Protonation" refers to a fundamental step in catalysis during which hydrogen attaches to molecules. "This is the important region of the protein, where the chemistry is happening and the chlorite is being broken down," Coates said.

Protonation states are not easily observed because they involve hydrogen, which is difficult to detect with X-rays or other techniques. In addition, a phenomenon called "photoreduction" occurs when metal-containing enzymes like chlorite dismutase are exposed to X-rays, essentially changing the atomic structure of the sample.

Because neutron techniques do not have these limitations, they can give researchers key information that cannot be obtained by other methods.

"Neutrons are nondestructive and sensitive to light elements like hydrogen, so they can provide exclusive information about the atomic structure of proteins, which are largely composed of hydrogen molecules," Coates explained. "And unlike X-rays that can damage delicate proteins, neutron techniques allow you to collect data at room temperature on an unaltered protein in its active state without the impacts of ionizing radiation and photoreduction.

"This experiment really highlights the benefit of using neutrons to study proteins," Coates said.



Chlorite dismutase is a unique oxygen-generating enzyme that degrades chlorite, an industrial pollutant found globally in groundwater, drinking water and soils. Journal cover art reprinted with permission from *ACS Catalysis*

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.

Patricia S. Langan

Postdoc, Neutron Scattering Division
Ph.D., Nanoscience and Microsystems Engineering, University of New Mexico
Hometown: Los Alamos, New Mexico

What are you working on at ORNL?

My research at ORNL includes probing the relationship between the structure and function of biological molecules, using neutrons at the Spallation Neutron Source. One project includes exploring the breakdown of antibiotics by beta-lactamases, enzymes that confer drug resistance to bacteria.

What would you like to do in your career?

I'd like to continue to do research that investigates the biological structure-function relationship and the molecular basis of disease, using a variety of methods.

Why did you choose a career in science?

I chose a career in science because I've always been interested in biology. I enjoy research and the excitement of a successful experiment, particularly when the results aren't what I expected!

Jordi Casanova

Postdoc, Physics Division
Ph.D., Astrophysics, Universitat Politècnica de Catalunya
Hometown: La Garriga, Spain

What are you working on at ORNL?

My work focuses on understanding the nature of stellar explosions, such as core-collapse supernovae and classical novae. Currently, I am performing multidimensional hydrodynamic simulations to study the interplay between turbulence and the dynamics of the explosion during a supernova event.

What would you like to do in your career?

I am a theoretical astrophysicist interested in deciphering how stars explode and die. I want to strengthen the connections among the research groups working on different aspects of stellar physics and develop novel techniques to finally construct a solid theory, aimed to describe these titanic explosions in the universe.

Why did you choose a career in science?

I have always been fascinated by the cosmos and wondered how the universe is structured. Becoming a scientist allows me to satisfy my curiosity about solving this puzzle and get excited by new findings every day. In the end, there is nothing more beautiful than stars.

Dongsook Chang

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Chemical Engineering, Massachusetts Institute of Technology
Hometown: Seoul, South Korea

What are you working on at ORNL?

I'm working on improving our understanding of polymer materials. I'm currently trying to answer questions about how polymer architecture affects the topology of chains at interfaces and how deuteration (the adding of heavy hydrogen) affects material properties such as crystallization and solubility.

What would you like to do in your career?

I'd like to continue to have opportunities to do exciting research on polymers either in an academic or industry setting.

Why did you choose a career in science?

Growing up, I was inspired by my father, who studied nuclear engineering. I also love learning new things and understanding the world better every day.

Vincent Heningburg

Graduate student, Computer Science and Mathematics Division
Ph.D. student, Mathematics, University of Tennessee
Hometown: Prattville, Alabama

What are you working on at ORNL?

I am working on numerical solutions to transport equations using the discrete-ordinates method. Transport equations are used to track particle densities within a medium, and their applications include nuclear reactor simulations and radiative shielding design. In particular, I am using filters to reduce the occurrence of nonphysical defects, known as "ray-effects," in which the discrete ordinates leave an imprint on the numerical solution.

What would you like to do in your career?

I would like to continue doing research in numerical solutions of various partial differential equations in the field of kinetic theory. I would also like to help develop better algorithms in a high-performance computing setting for solving the type of equations seen in kinetic theory.

Why did you choose a career in science?

Science has been an interest of mine since I was very young. The idea of discovering something new about the universe through problem solving had a certain appeal. It was my undergraduate adviser who sparked an interest in math in particular. I get a rush out of proving a difficult theorem or when my algorithms produce reliable results.

Victoria DiStefano

Graduate student, Chemical Sciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Chattanooga, Tennessee

What are you working on at ORNL?

My research seeks to improve the efficiency of oil and gas extraction in hydraulic fracturing by determining how oil and gas are stored in gas shales. I use highly penetrating neutrons to determine the location, type and amount of organic matter stored in shale pores.

What would you like to do in your career?

I would like to work on creative solutions to the energy issues facing our nation. I hope to use my knowledge of energy systems, and the complex problems associated with them, to inform national and regional policies of energy production, distribution and management.

Why did you choose a career in science?

I chose a career in science to help understand and solve the fundamental problems of our energy system, ensuring reliable and equitable access to energy resources. I was also inspired by my grandfathers, Jim DiStefano and Harley Ross, both of whom where researchers at ORNL and encouraged my love of science.

Jesse Piburn

Graduate student, Computational Science and Engineering Division
Ph.D. student, Data Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Gallatin, Tennessee

What are you working on at ORNL?

I use data science to help answer questions related to socioeconomic development, urban dynamics, clean energy and other interesting domains. My background is in spatial statistics and geographic information science, so most of what I am currently working on has a strong geographic or spatial component.

What would you like to do in your career?

Throughout my career, I want to be in a position where my abilities can make the largest contribution to science and the organization I am a part of. Currently that means finishing my Ph.D., but in the future, whether in a project or line management position, I would like to lead a team of scientists and engineers.

Why did you choose a career in science?

I have always had a passion for learning new things. Having a career in science allows me to pursue that passion while contributing to the scientific community. In particular, working here at ORNL ensures that not only do I have a career in science but also a career where I can help solve real-world problems.

ORNL dips a toe into artificial intelligence

by Tim Gawne
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Most of us grew up watching TV and movies that depicted artificial intelligence in a less than comforting light. From 1927's "Metropolis" to last year's "Blade Runner 2049," Hollywood has imagined AI as a force for threatening the world, enslaving humanity and being an all-around bad actor.

These destructive, self-aware machines make for excellent theater, of course, but they obscure the benefits we stand to gain from AI, especially in research. Even as the capabilities of computing and data analysis ballooned over the decades, people often had difficulty distinguishing real AI from the killer robots of the silver screen.

"It is always interesting to observe the response of an audience introduced to the research field called 'artificial intelligence,'" ORNL AI pioneer Carroll Johnson noted in 1981. "The very term implies that a computer can be programed to reason like a person. The concept may seem frightening, preposterous or stimulating depending upon the listener's viewpoint, and these reactions are often reflected in the comments from the audience."

Johnson launched the lab's earliest AI effort after returning in 1976 from a sabbatical at Stanford University. Stanford had developed CRYSALIS, an AI effort that infers the atomic structure of protein molecules, and Johnson helped guide that effort with his expertise in crystallography.

In October 1979 he assembled a panel of ORNL researchers—both domain scientists and computer engineers—to launch the Oak Ridge Applied Artificial Intelligence Project. Its goal: to evaluate AI as a tool for supercharging research at the lab.

One panel member was Michelle Buchanan, then an early career analytical chemist, now the lab's deputy for science and technology. Buchanan worked with software called EXPERT, developed at Rutgers University for use in spectroscopy.

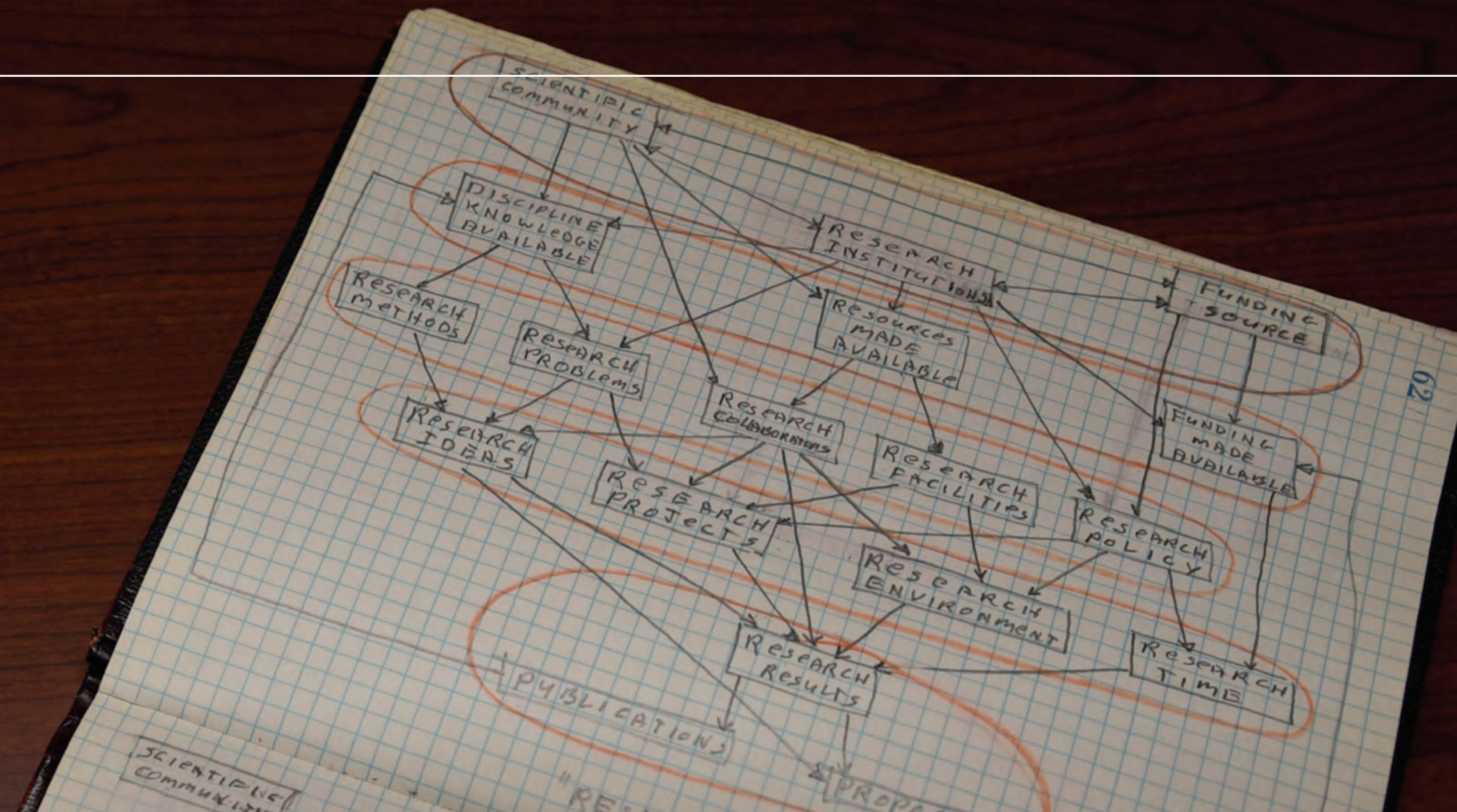
Buchanan says the project remains one of the most rewarding activities of her career at the lab. She recalls the meticulous interviews Johnson would set up to capture the interpretation of infrared, nuclear magnetic resonance and mass spectral data. This attention to detail led Johnson to produce nearly 1,500 pages of notes.

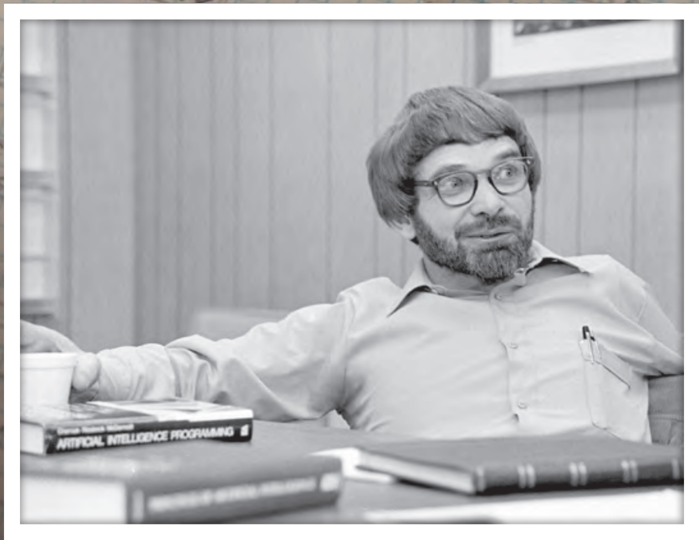
Johnson saw the potential for an AI system like the adapted EXPERT to work with a computer-controlled instrument such as a mass spectrometer and provide real-time data capture and analysis.

In 1981, participants in ORNL's early AI efforts included, from left, John Allen, a consultant from ProPhysica Inc., ORNL spectroscopy expert (and current deputy of science and technology) Michelle Buchanan, and Sara Jordan, a University of Tennessee professor and ORNL researcher.

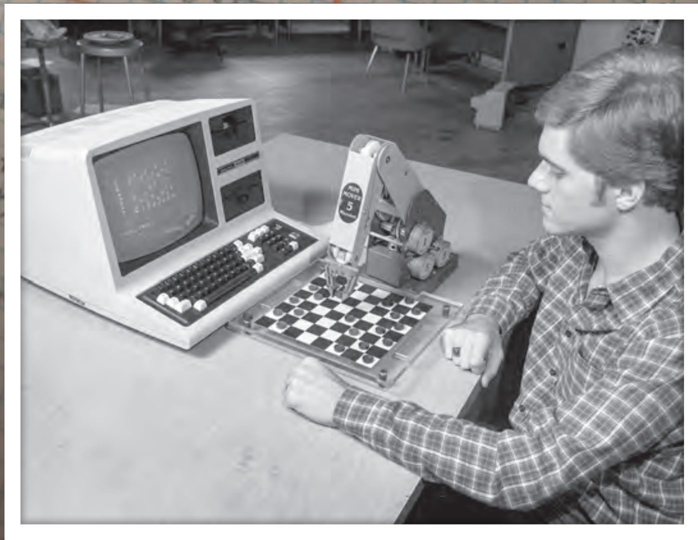
For those reading Johnson's notes, the concepts, principles and domains of potential application are not that far removed from our aspirations today. The only observable difference appears to be the scale of both the applications being deployed and the systems on which they are deployed. ORNL's Titan supercomputer—a Cray XK7—is more than 150 million times faster than Cray's flagship system at the time Johnson formed his panel in 1979.

With this greater capacity, we are seeing Johnson's dream become reality.





ORNL AI pioneer Carroll Johnson in a 1981 photo from ORNL Review.



University of Tennessee engineering student Tom Swift demonstrates a simple program showing that a robot arm can avoid obstacles in this 1984 photo from ORNL Review.

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

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Oak Ridge National Laboratory is managed by
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DE-AC05-00OR22725

ISSN 0048-1262