

ARGONNE | NOW

VOLUME 06 / ISSUE 01 / SUMMER 2012

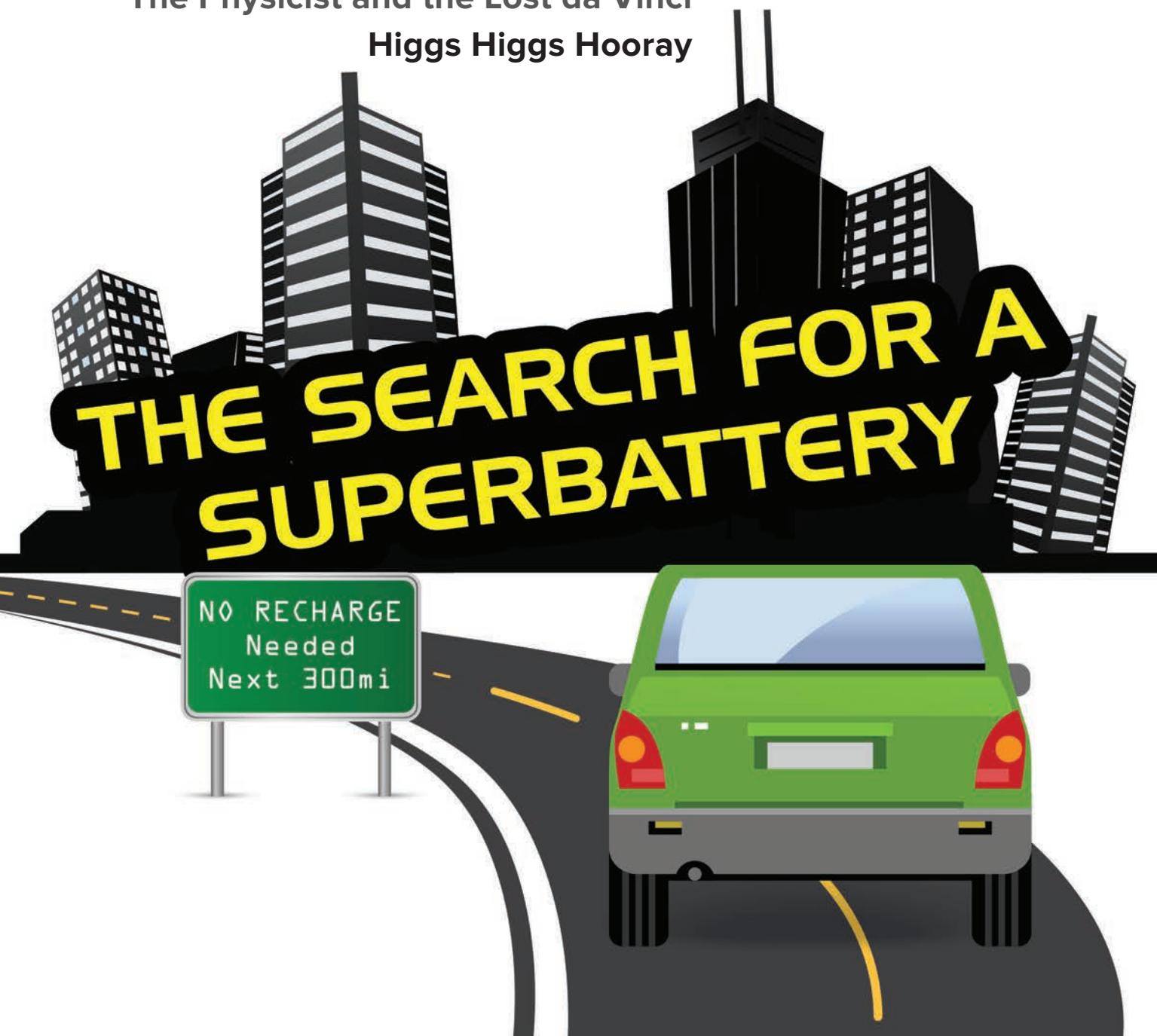
Inside the Advanced Photon Source

Meet Our New Supercomputer

Preparing for Pandemic Flu

The Physicist and the Lost da Vinci

Higgs Higgs Hooray



ARGONNE NOW

editor

Louise Lerner

editorial board

Ed Daniels
Rick Fenner
Robin Graham
Matt Howard
Denny Mills
Michael Papka
Mark Peters
Cosmas Zachos

photography

Wes Agresta
George Joch

art and design

Sana Sandler

production

Gary Weidner

send correspondence and questions to:

Argonne Now
Communications & Public Affairs
Building 201
Argonne National Laboratory
9700 S. Cass Avenue Argonne, IL 60439

argonnenow@anl.gov
630 252 5526

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC. The laboratory's main facility is outside Chicago at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see www.anl.gov.

disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Sign up to receive your copy of *Argonne Now* at www.anl.gov/subscribe



Dear Reader,

Here at Argonne, our scientists and engineers are tightly focused on our mission of discovery and innovation in the national interest. We work each day to find new sources of clean energy, stretch the boundaries of scientific discovery, and create new technologies that can recharge our economy. Our research is important, compelling, and potentially game-changing, and we welcome

finding new ways to share the work we do here with the larger community.

So as Director of Argonne, I am very excited to present this relaunch of *Argonne Now*, our semi-annual laboratory magazine. As you will see, we are adding more pages of science and engineering news. We also are offering a number of special features, including this issue's review of educational opportunities at Argonne and our look at the real science (or lack of it) that underlies contemporary movies and television shows.

I recommend our cover story, "The Search for a Superbattery," which follows Argonne's quest to develop a lithium-ion battery with the muscle to power a car for 300 miles or more on a single charge. The story begins in Argonne's materials science division and takes you all the way to the new generation of electric vehicles on the road today. But the story doesn't stop there: we continue to develop better ways to make advanced batteries that can make electrical cars safer, more reliable, and more affordable.

In this issue, you'll meet "Mira," our laboratory's powerful new supercomputer, you'll see what our scientists are discovering at the Advanced Photon Source (one of the world's leading synchrotron light sources), and you'll find out how we helped Chicago prepare for a potential pandemic flu outbreak.

We want you to have a voice in this new magazine as well. Are you wondering about dark energy and why it's so important to our understanding of the universe? You can ask a scientist on page 66.

To stay connected with the laboratory's work between issues of *Argonne Now*, we invite you to sign up for our monthly email newsletter, *Argonne Advances*, and to follow us on Facebook and Twitter.

We hope you'll enjoy this new *Argonne Now*, and we look forward to hearing from you.

Eric D. Isaacs, Director

Argonne provides scientific and engineering solutions to the grand challenges of our time: sustainable energy, a healthy environment, and a secure nation.

in this issue

NEWS

- 8 [Mapping Underground Waterways with Krypton-81](#)
A rare isotope tracks how long water has been underground.
- 9 [From the Ground Up](#)
The University of Chicago dreams small with its new Institute for Molecular Engineering.
- 10 [Biochips for Bovines](#)
A chip to diagnose cattle disease wins an entrepreneurial challenge.
- 11 [Untangling the Mysteries of Spider Silk](#)
Powerful X-rays reveal the atomic structure of spider silk.
- 12 [Higgs, Higgs, Hooray](#)
Argonne scientists help track down Nature's most elusive particle.
- 14 [Don't Sweat the Flu](#)
The City of Chicago drills its staff for a pandemic flu outbreak.
- 16 [The Physicist and the Lost Da Vinci](#)
An Argonne scientist thinks he can find out whether a lost masterpiece is hidden behind a 500-year-old wall.
- 20 [The Minimal Microbe](#)
How many genes can you strip from a cell and still call it a cell?
- 22 [A Natural Solution for Transportation](#)
Compressed natural gas offers an alternative to gasoline.
- 24 [SHARP Thinking](#)
Computing could shave millions off nuclear reactor design costs.

FEATURES

- 26 [INTRODUCING MIRA](#)
Meet Argonne's new 10-petaflop supercomputer.
- 32 [THE SEARCH FOR A SUPERBATTERY](#)
Research at Argonne will help power the next generation of electric vehicles.
- 38 [INSIDE THE ADVANCED PHOTON SOURCE](#)
Access the atomic level at Argonne's giant synchrotron.

SHORTS

- 42 [7 Things About Catalysis](#)
Learn about the mysterious agents that make your beer, bread, paper, and plastic.
- 46 [Book Review: Bottled Lightning](#)
Director Eric Isaacs reviews *Popular Science* writer Seth Fletcher's latest on lithium-ion batteries.
- 50 [Argonne in the Marketplace](#)
Thin sheets of diamonds have worlds of uses.
- 52 [The Secret Lives of Nuclear Scientists](#)
Among the 1,400+ scientists at Argonne are a *Breaking Bad* actor and an award-winning chef.
- 54 [Chasing a Common Cold Virus](#)
Adenoviruses are spiky, tricky creatures, but scientists are shedding light on their structures.
- 56 [Education at Argonne](#)
Learn about some of the opportunities for students at Argonne.
- 60 [Greening the Campus](#)
Argonne's visitor center is now cooled by pipes that go 600 feet underground.
- 61 [Coming to Campus](#)
Take a peek at two new buildings under construction at Argonne.
- 62 [Science Behind the Fiction: Contagion](#)
How accurate is *Contagion's* killer virus outbreak? Argonne emergency planners weigh in.
- 66 [Ask a Scientist: Battery Life](#)
Is it true that running my battery all the way down makes it last longer?
- 67 [Science Haiku](#)

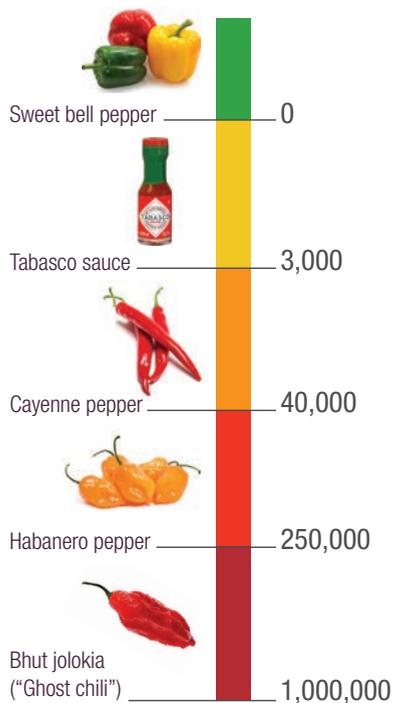
Science History

100 YEARS AGO

1912 – How Hot?

Wilbur Scoville invents a test to measure the hotness of peppers. The human tongue was still a much more accurate detector than any lab technique at the time, so his test measures how much a pepper has to be diluted before it can't be tasted anymore. Your tongue can detect the heat, a molecule called capsaicin, at a concentration as low as 10 parts per million. The test has since been replaced with more precise lab techniques, but pepper heat is still often rated in Scoville units.

How Many SCOVILLE Units?



66 YEARS AGO

1946 – Happy Birthday Argonne

Argonne was chartered as the first national lab in 1946. Its mission: harness the power of the atom for peaceful energy generation. Today, the lab conducts science and engineering research to solve problems in energy, environment, and national security.

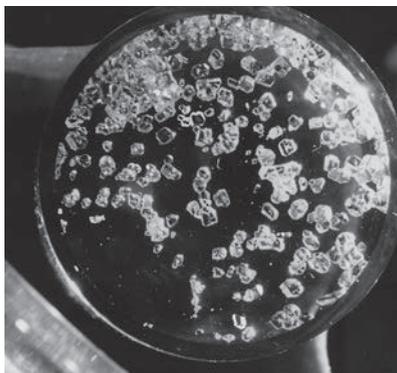


Albert Crewe (right), Argonne director from 1961 to 1967, stands next to the lab's Cockcroft-Walton generator.

50 YEARS AGO

1962 – A New Bond

Argonne scientists announce that they have created a compound with xenon, one of the noble and inert gases once thought too stable to form any compound. The creation opened a new era for the study of chemical bonds.

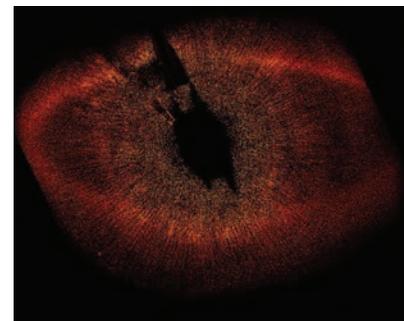


Crystals of xenon tetrafluoride

20 YEARS AGO

1992 – A Planet Far, Far Away

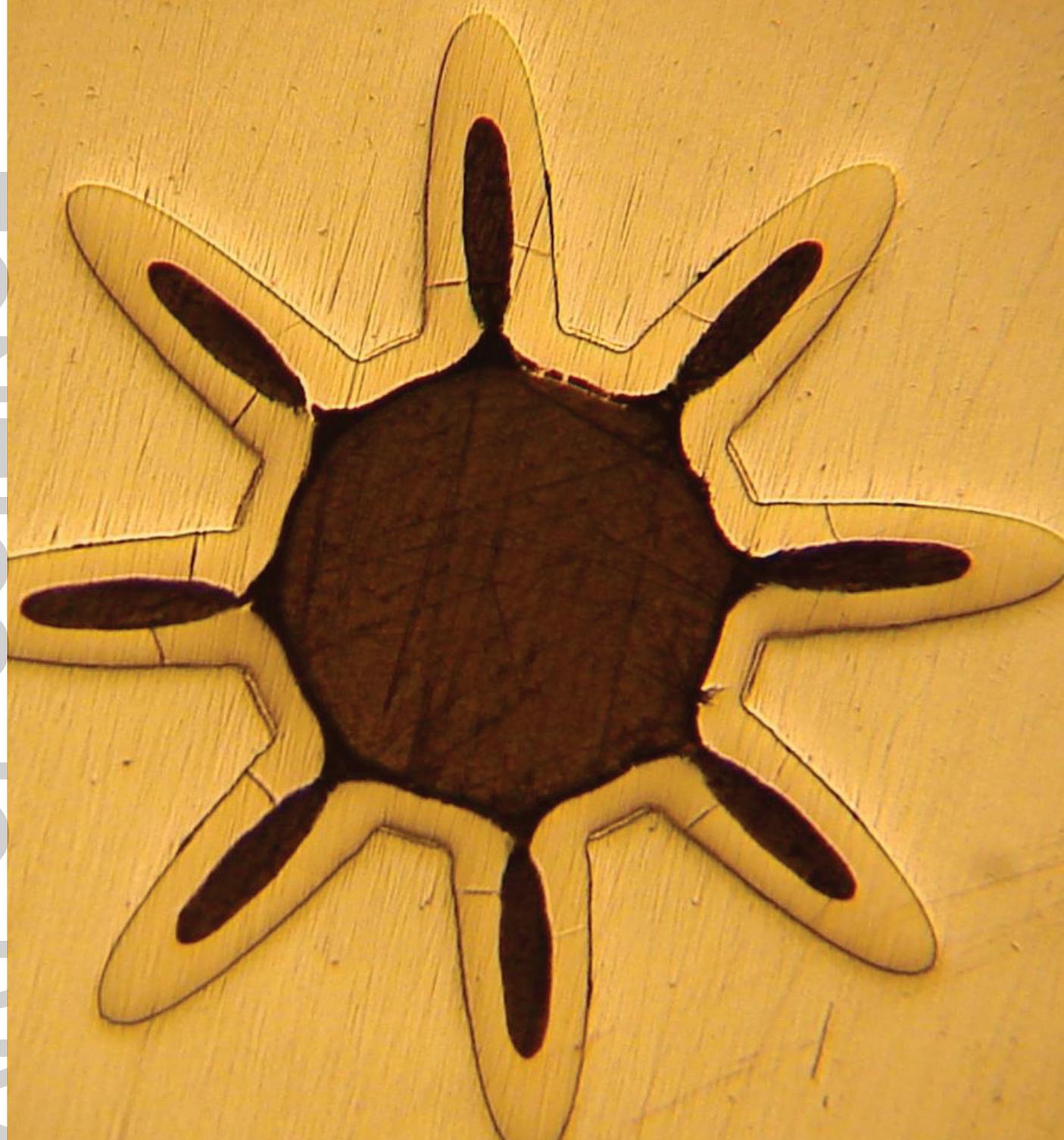
The first planets ever discovered in another solar system are found by astronomers Aleksander Wolszczan and Dale Frail. The planets orbit a neutron star in the constellation Virgo, roughly 2,000 light-years away. Today scientists have identified more than 700 extrasolar planets.



NASA, European Space Agency, and P. Kalas (University of California, Berkeley)

history
Science History

ART OF SCIENCE



Fuel injector flower

By Nicholaos Demas

The nozzle of the fuel injector in a car sprays gasoline through tiny holes, designed to make as fine a mist as possible so that the fuel burns better. Researchers at Argonne, attempting to make the engine even more efficient, reduced the size of the holes to less than the diameter of a single human hair. This is a nozzle with eight holes—polished from the tip down to reveal a flower-like pattern—seen under a microscope. The dark areas are the holes, the yellow area is the iron nozzle, and the petals are the nickel-phosphorous material used to reduce the size of the holes.

Mapping underground waterways with

by Louise Lerner



KRYPTON-81

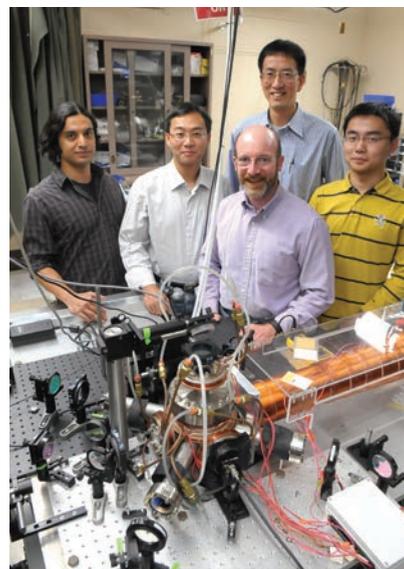
Cataloguing underground waterways, some of which extend for thousands of miles, has always been difficult—but scientists at Argonne, with colleagues from the University of Illinois at Chicago and the International Atomic Energy Agency, are mapping them with some unusual equipment: lasers and a rare isotope.

About a fifth of people on Earth drink water drawn from underground, and crops around the world depend on it; experts believe that aquifer depletion contributed to the worldwide food shortages last year. Underground water is less prone to pollution and is the only source of water in many dry areas where surface water quickly evaporates.

Water accumulates in aquifers only after filtering slowly through sand and cracks in rocks, which can take millennia in some areas. In order to manage this resource fairly and effectively, consumers need to know how fast the water is replenished.

But because the areas that feed aquifers can extend for thousands of square miles—and conditions over any of those areas affect

them—it's been difficult to get an accurate model of the entire system. Good models could predict water availability according to changes in vegetation, terrain, rain, droughts, or monsoons.



Argonne physicist Zheng-Tian Lu (in back) and his team (from left to right: Arjun Sharma, Wei Jiang, Kevin Bailey, Guomin Yang) stand with the ATTA device.

What scientists needed to improve their models was a way to calculate the “age” of the water, or how long the water has been underground.

When water spends time above ground, it picks up tiny traces of isotopes that are naturally present in the air. One of these is krypton-81,

an atom that decays extremely slowly. The technique is similar to carbon dating done on fossils: if you know how slowly Kr-81 decays and can count the remaining Kr-81 atoms in the water, you can calculate how long it's been since the water was above ground.

Scientists have been hoping for a way to use Kr-81 for dating since the 1960s; it's a remarkably long-lived isotope that can be used to date back much further than carbon—perhaps as far back as a million years. But since the isotope is extremely rare in the atmosphere, researchers needed a way to measure incredibly small amounts of atoms.

Laser trapping and cooling of atoms, an area of physics pioneered by Energy Secretary Steven Chu, turned out to be the answer. Argonne physicist Zheng-Tian Lu leads a team that has worked since 1997 to adapt Chu's atom trap to count individual atoms of Kr-81. The result is called Atom Trap Trace Analysis (ATTA), which combines lasers with a camera to image atoms.

The device uses a chamber with six laser beams to capture individual atoms. To set the trap to catch only Kr-81 isotopes, scientists tune the lasers' frequencies to match the specific resonances of Kr-81 atoms.

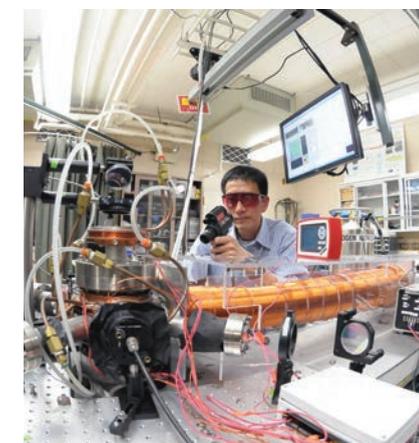
This research was supported by the Department of Energy's Office of Nuclear Physics and by the National Science Foundation.

Atoms vibrate at frequencies that are specific to each isotope. When they're hit by resonant light, they become excited and vibrate faster—and show up as a bright spot on the camera.

Lu partnered with University of Illinois at Chicago geologist Neil Sturchio to use ATTA in a sample study to determine the age of the Nubian Aquifer in the Sahara Desert. The analysis agreed with independent hydrodynamic models, confirming the flow of water toward the northeast and even indicating

flow rates of approximately one meter per year.

Both Lu and Sturchio are now partnering with Pradeep Aggarwal, who leads the Isotope Hydrology Section at the International Atomic Energy Agency, to conduct a larger-scale study. The team collected samples in Brazil last year, which were sent to Argonne for analysis. If the study proves successful, the technique could be used to map aquifers and groundwater all over the world. ☼



Zheng-Tian Lu adjusts the ATTA device.

UNIVERSITY OF CHICAGO New institute to study molecular engineering



When completed in early 2015, the William Eckhardt Research Center will house the Institute for Molecular Engineering at the University of Chicago.

Matthew Tirrell studies micelles, collections of lipid molecules that form spontaneously in water. The founding Pritzker Director of the Institute for Molecular Engineering at the University of Chicago, Tirrell has developed a type of micelle that, when injected into mice, migrates to the location of artery-hardening plaque. Using that homing capability, he says, scientists could tailor micelles for diagnostic or therapeutic uses—dissolving blood clots, for example, or delivering medication to treat a tumor.

Designing structures to achieve such ends involves a process called molecular self-assembly. “When you put things together in a beaker, they don't chemically react,” Tirrell says, “but they spontaneously organize into structures that are useful.”

He wants the new Institute for Molecular Engineering to operate with

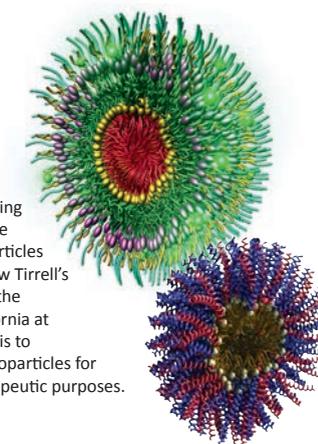
similar spontaneity. Faculty members will be encouraged to organize themselves into problem-solving teams.

“I want people that are broad and versatile enough to think about applications not only in health care but energy, environment, maybe even in computing: how does biology transform information? Stuff like that,” Tirrell says. “That's going to mean that we're going to have people skilled in biology working with people skilled in electrical engineering—unusual combinations.”

The institute is partnered with Argonne; three new hires named this

summer have joint appointments with the university and the lab. Over the next several years, the faculty will grow to about 25.

“The IME will have a kind of license to do things together the way a research institute does and a license to acquire faculty the way an academic unit does,” Tirrell says. “That doesn't exist elsewhere as far as I know. We're not going to have departments, we're not going to divide ourselves up; we're going to emphasize coming together to solve big problems.”



Nanoparticle

This artistic rendering depicts some of the circulating nanoparticles studied by Matthew Tirrell's research group at the University of California at Berkeley. The goal is to engineer such nanoparticles for diagnostic or therapeutic purposes.

—compiled from *The University of Chicago Magazine*

BIOCHIPS FOR BOVINES

TECH FOR CATTLE DISEASE WINS ENTREPRENEURIAL CHALLENGE

by Louise Lerner

NEW VENTURE CHALLENGE

SiteDiagnostics, a start-up biotechnology company based on biochip research by Aeraj ul Haque and Dan Schabacker, won fourth place in the 2012 Edward L. Kaplan, '71, New Venture Challenge. The challenge is a business creation competition that funds the best entrepreneurial ideas by students at the University of Chicago's Booth School of Business.

The start-up will receive \$10,000, office space at the University of Chicago for the summer of 2012 and networking opportunities, part of the Polsky Center Summer Accelerator Program. Using the award, ul Haque and Schabacker plan to find farms to start initial tests of the technology. They also want to further reduce the cost of each chip from about \$8 to \$5.



Argonne scientists are feeling bullish about new biochips that can diagnose bovine mastitis infection in dairy cows.

Bovine mastitis is an udder inflammation that can put a cow out of commission for months. It costs the dairy industry \$10 billion worldwide every year, said Argonne postdoctoral researcher Aeraj ul Haque, and can be caused by several different bacteria.



Argonne scientists Aeraj ul Haque (left) and Dan Schabacker developed a biochip to diagnose bovine mastitis.

“Knowing the cause is really helpful to the farmer, because different causes have different treatments,” ul Haque said.

Currently, farmers have tests to determine whether a cow has mastitis, but not which bacterium is causing it. That's where the chip comes in.

Based on technology originally developed for national security applications, the biochip contains tiny wells, each holding an antibody that recognizes a specific piece of a bacterium. The farmer applies a sample of milk from an infected cow to the biochip; if one of the antibodies latches on to a pathogen, that well turns blue.

“The same six bugs account for close to 90% of all mastitis cases,” ul Haque explained, which makes a chip practical since antibodies for many common bacteria are already commercially available.

“We could also adapt this to detect quite a few other diseases in other veterinary applications,” he said. “Bovine tuberculosis, canine heartworm disease, even mad cow. Anything with a proteomic biomarker, we can detect.”

UNTANGLING THE MYSTERIES OF SPIDER SILK

by Jared Sagoff

Spiders weave a web even more tangled than originally thought—at least on the nanoscale level, according to new studies at Argonne.

Using X-rays from the Advanced Photon Source (see page 38), scientists peered into the structure of orb spiders' dragline silk. This is the chief thread that allows them to dangle precipitously off branches and window frames.

“Spider silk has a unique combination of mechanical strength and elasticity that makes it one of the toughest materials we know,” said Professor Jeffery Yarger of Arizona State University, one of the lead researchers of the study.

The inner core of dragline silk is made up of a set of tiny fibers called fibrils, which, at the atomic level, organize into two different regions. The incredible strength of the material comes from crystalline lattices that compose roughly 10% percent of the total webbing, while its elasticity is the result of so-called “amorphous” regions that make up the remaining 90%.

Argonne X-ray scientist Chris Benmore developed an experiment to probe the nanocrystalline structure of dragline spider silk. According to Benmore, previous studies of spider silk focused on the crystalline regions because their structures were easier to image. “In this study, we focused on getting a good view of the amorphous



Left: A *Nephila clavipes* female spider in the center of her web. The radial strands and scaffolding of her web are composed of major and minor ampullate spider silk fibers. Commonly referred to as dragline silk, this substance was imaged at the nanoscale at Argonne's Advanced Photon Source. Image by Jeff Yarger.

areas, which is something you really need a machine like the APS for,” Benmore explained.

Unlike the crystalline areas, which tend to arrange themselves in predictable patterns, the scientists found that the atoms in the amorphous parts of dragline silk lost their ordering after about a nanometer.

By getting a better picture of the relationship between the amorphous and crystalline structure of natural silks, Benmore and Yarger hope to provide the grounds for simulations that could improve a whole class of synthetic materials, including artificial spider silk.



by Jared Sagoff

HIGGS, HIGGS, HOORAY

Argonne scientists help track down Nature's most elusive particle

On July 4, as fireworks exploded across the United States in celebration of Independence Day, scientists around the world also began to celebrate what is widely considered the biggest experimental achievement in physics in decades.

At the Large Hadron Collider in Geneva, Switzerland, scientists associated with two different experiments independently confirmed the detection of a new particle thought to be the Higgs boson—a result that would give credence to a theory devised almost 50 years earlier.

In 1964, a young physicist named Peter Higgs published a theory that postulated the existence of a new fundamental particle that would answer some of the biggest questions in physics. Why did electrons, for instance, have mass when theory suggested that they should have been massless?

The answer, Higgs thought, lay in the existence of an invisible field that permeated the entire universe, even vacuums. He suggested that particles gain mass by passing through the field.

How does one find an invisible field? Physicists believe that the field manifests itself as a tiny, extremely unstable particle that decays almost instantaneously. The trick was getting the right conditions: an accelerator that would smash protons together at high enough energies to produce the particle.

“To give you kind of an idea of the sorts of scales we're talking about, if an atom were the size

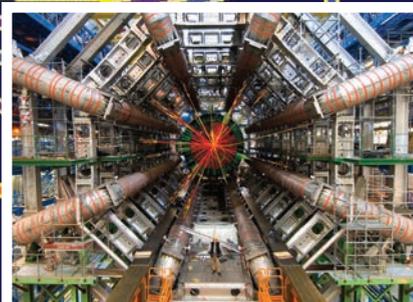
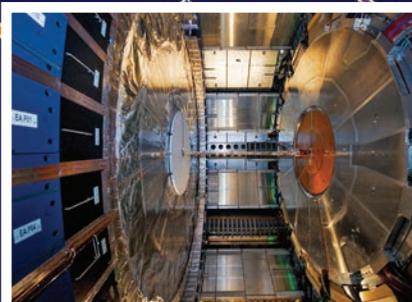
of the Earth, the particles we're looking right now are at the scale of a pea,” said Argonne physicist Tom LeCompte, who served as the physics coordinator at one of the project's major experiments.

Since it came online in 2008, the nearly 17-mile-long collider has housed two parallel hunts to detect signs of the Higgs. Argonne helped build detectors for one of the two experiments, known as ATLAS, and scientists from the laboratory have worked to enable massive data sharing via grid computing, oversee experiments, and analyze the results.

“The results presented today are the outcome of over 20 years of effort by several thousand scientists throughout the world, and Argonne's contributions to the ATLAS detector made possible the acquisition of the data we're discussing today,” said Argonne senior physicist James Proudfoot. “This is a historic milestone—but only the beginning as we start the task of exploring the properties of this new particle.”

The pinpointing of a Higgs-like particle does not mean that high-energy physicists now have all the answers.

“There are still many unanswered questions in high-energy physics, and the conclusions we've drawn from the data we've gathered open up as many new questions as they begin to settle,” LeCompte said. “I'm certain we'll get much, much closer soon, though. There's no way out for Nature. We've got her closed in on all sides.”



City of Chicago won't sweat the flu with Argonne's help

by Louise Lerner



Last year, officials at Chicago's Department of Public Health watched the H5N1 bird flu tear through neighborhoods, taking down public agencies and shuttering public schools.

Good thing it was just a drill. Emergency preparedness experts at Argonne have helped the Chicago department plan its response to potential catastrophe, including swine and bird flu epidemics, plague outbreaks, and anthrax bioterrorism.

Chicago, as one of the four largest cities in the nation, is required by the U.S. Centers for Disease Control and Prevention (CDC) to run periodic exercises demonstrating how effectively it would respond to public health emergencies. Local hospitals often join the exercises, as does the city's Office of Emergency Management and Communication. Even O'Hare Airport, a likely gateway for viruses from around the world, has played along in the past.

For the H5N1 flu exercise, the Argonne team served as architects and built the scenario into a computer planning tool that helped guide the exercise and track city agencies' responses.

After carefully planning out the spread of the "flu attack," they launched the scenario. Over a three-day period, at specific points, they fed information to the Chicago department about the spread of the flu and watched the results unfold.

"We start off slow, but by the third day, the city is reeling—influenza cases, workforce shortages, laboratory samples, requests for media interviews and news conferences," said Dan Walsh, an emergency preparedness specialist at Argonne. "We like to keep them on their toes."

This particular exercise followed the spread of an imaginary flu from Egypt. By the time the flu "arrived" in Chicago, more than 15,000 cases had been reported worldwide. Reports of an outbreak at an area nursing home kicked off the Chicago

scenario. City officials face a cascade of difficult decisions. Do they cancel trade shows? Close the Chicago Public Schools? Quarantine travelers at O'Hare Airport? Ask churches, temples, and mosques to suspend services?

Argonne's emergency preparedness experts have collaborated with the Chicago Department of Public Health (CDPH) to run more than 20 exercises over the past few years, for scenarios ranging from pandemics to bioterrorism to heat waves. After creating the scenario, the team helps control the flow of the exercise by sending new information and challenges, monitors the drill, and offers suggestions for improvement at the conclusion.

The exercises are designed to be "no-fault"—no one is disciplined as a result. "We emphasize to the participants that it is OK to make mistakes during a drill as long as they use the lessons learned to improve preparedness and



response levels before an actual event," Walsh explained.

Walsh said the team makes sure to throw wrenches in the works, to mimic the unpredictability of real-life scenarios. For example, in the last drill, the CDPH computers "malfunctioned," forcing the department to operate without computer assistance for several hours. Another day found emergency staff refusing to work unless they received masks and vaccinations first and McCormick Place officials challenging the city's decision to ban large public gatherings.

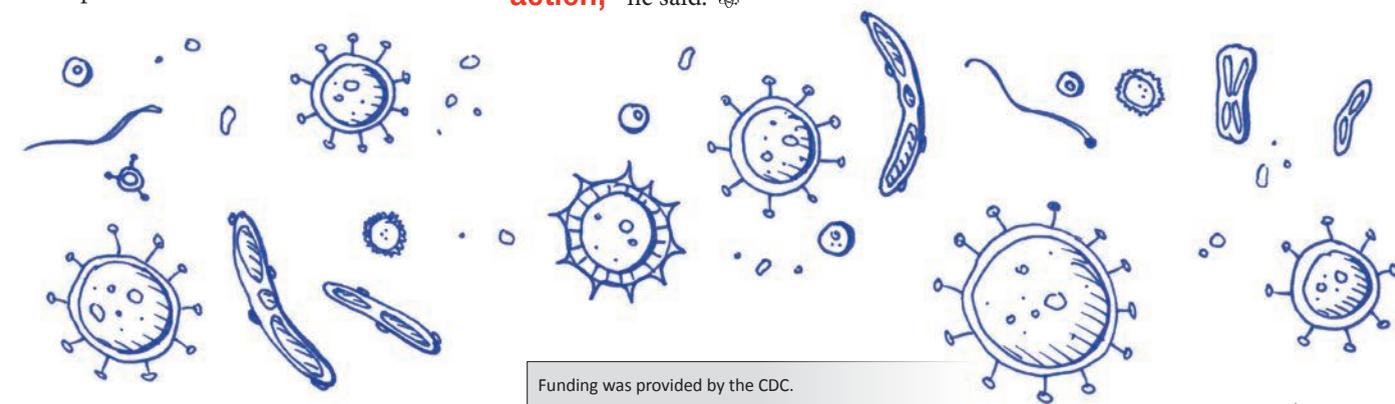
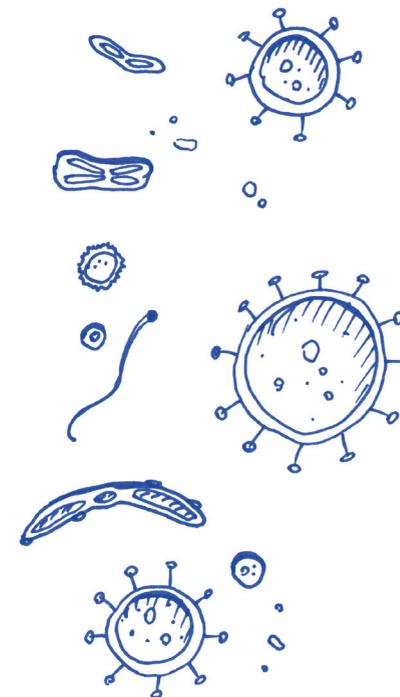
Argonne experts even pose as reporters at mock news conferences, pressing the officials for information. To make the scenario seem even more real, the risk communications team produced 22 video, radio, and print news stories to match the

media intensity in real emergencies.

The planning tool, called the Sync Matrix Enterprise, was developed by Argonne's Decision and Information Sciences division and allows Argonne experts to coordinate with CDPH officials to plan, control, and evaluate the exercises.

"The process has proved very helpful in our real-life response to the H5N1 flu; by the time the virus hit, we'd already had two years of planning exercises with Argonne," said Ed LeFevour, CDPH manager of emergency management services. "We held a planning session just a few weeks before we went live with 100,000 H5N1 vaccinations in the Chicago area.

"The community is better prepared as a result of this action," he said.



Funding was provided by the CDC.

The Physicist and the Lost da Vinci

by Louise Lerner

Could an Argonne scientist detect a long-lost painting behind a 500-year-old wall?



All photos courtesy Dave Yoder/National Geographic Society.

Perhaps one of Leonardo da Vinci's greatest paintings has never been reprinted in books of his art. Known as the "Battle of Anghiari," it was abandoned and then lost—until a determined Italian engineer gave the art world hope that it still existed, and a physicist from Argonne National Laboratory developed a technique that may reveal it to the world once again.

The story starts in 1503 in the newly constructed "Hall of 500" of the Palazzo Vecchio, the town hall of Florence, Italy, where the city had called the geniuses Leonardo da Vinci and Michelangelo to each paint one wall. Leonardo chose to paint the

Battle of Anghiari, and his sketches promised a marvel of motion and color worthy of his best work.

Leonardo worked out the sketches while his assistants covered the stone wall with a coating to even out the surface and seal out moisture, probably a combination of gypsum and rosin. Next came a layer of cheap white paint, most likely a compound called "tin white" containing tin and linseed oil. Then the assistants would have taken his enormous sketch and transferred the outlines onto the wall.

Faced with a wall this large, most other painters of the day would have used the fresco technique: applying watercolor paints to wet plaster, which dries in a few hours. Leonardo, however, wanted to

experiment with oil paints, which allow for greater control, brightness, and layering of color—but dry painfully slowly.

He began painting, the layers most likely taking weeks to dry. But something went wrong. Accounts vary, some saying the paint didn't adhere well enough, others that the mixture was too thick and began to drip down the walls—or even that he tried to dry one section with charcoal braziers that melted the paint. Leonardo was called back to Rome for another project and abandoned the painting in 1505.

It sat half-finished for decades. Other artists flocked to the spot to study the remarkable painting; Raphael and Rubens, among others,

Above: Behind these frescoes may lie a half-finished masterpiece by Leonardo da Vinci. Left: Argonne's Robert Smither works with Italian collaborators on tests that could reveal the painting's presence.

made copies based on the drawing and subsequent engravings, which are the only images that survive.

Then the hall was remodeled in 1563, and fresco painter Giorgio Vasari was commissioned to cover the walls in frescoes. To do so, he had to paint over Leonardo's work.

Fast-forward 400 years, during which Vasari's frescoes became famous in their own right and art scholars labeled Leonardo's original work "lost." Until Maurizio Seracini, engineer and Leonardo enthusiast, stood in the hall in 1975 and noticed a tiny painted flag in Vasari's intricate battle scene with the message "CERCA TROVA:"

Seek and ye shall find.

Seracini speculated that the fresco painter might have constructed a brick second wall for his own work, leaving a few centimeters of space for Leonardo's sketch hidden beneath. At the time, however, technology did not permit exhaustive analysis. It wasn't until 2000 that Seracini returned, armed with laser and radar techniques, and confirmed the existence of a second wall.

Sonar, infrared, and radar can find hidden architecture, but they don't have the resolution to detect layers as thin as paint. Thus, Seracini had a problem. Since the Vasari fresco above it is also historic, the Italian government permitted Seracini to look for the painting but not to

touch the wall itself. He needed a noninvasive way to detect the painting.

Along the way, photographer Dave Yoder had picked up an interest in the project. Reading about imaging from a distance, he came across a paper by Argonne physicist Robert Smither, who had designed a crystal lens to look inside the human body without damaging it—why not a brick wall?

Smither suggested a method using neutrons as a "camera" to detect the existence of the painting. In this approach, a small generator would shoot beams of energetic neutrons at the wall where the painting might be hidden. Some neutrons would pass

NEWS

through the frescoes and brick wall and strike the layers of Leonardo's paint below. The neutrons would react with the metals in the oil paints, producing radioactive nuclei that emit characteristic gamma rays. Some of these gamma rays would pass back through the brick wall, where Smither would measure them with a detector.

"What we'd do is look for specific kinds of radioactivity produced by different color paints," Smither said.

Chemicals used for oil paint colors contain unique isotopes. For example, red paint would contain mercury sulfide, and the gamma rays coming from mercury sulfide have a

specific energy and decay rate, which the detector can measure.

"We think it should be possible to detect whether paint from the original painting survives, and perhaps even map an outline of the painting based on the colors," Smither said.

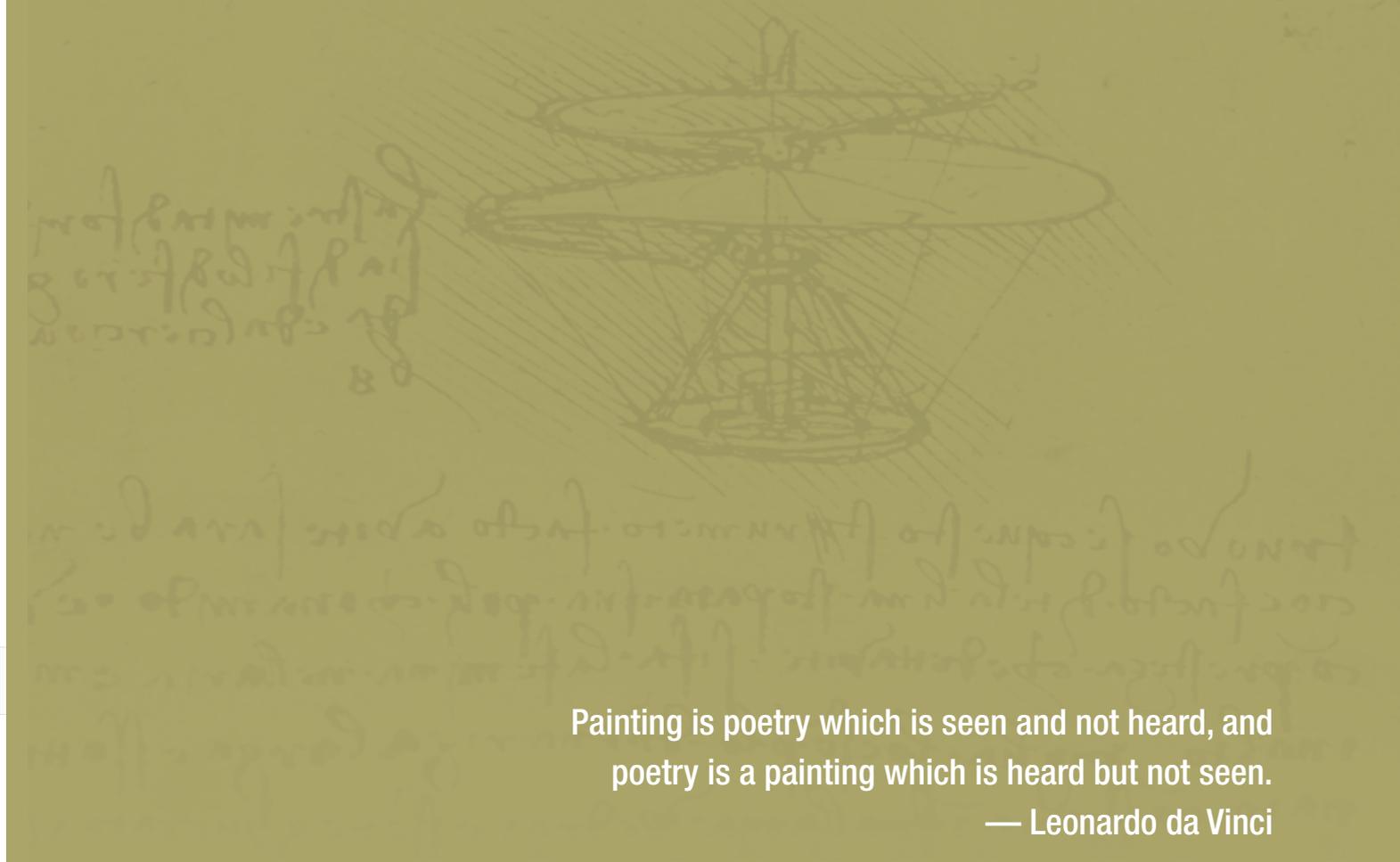
If no paint is detected, Smither says, the sadder alternative will be to beam the neutrons along the bottom of the opening to see whether Leonardo's paint flaked off the wall and collected at the bottom of the gap between the walls. (Half a millennium of weather—especially humidity—can devastate unprotected paintings, even those

hidden behind brick walls.)

Smither's preliminary tests have indicated that the gamma ray detector can indeed pick up signatures from paint from behind a brick wall. The hall itself presents its own challenges—the painting is 20 feet off the floor, and the neutron generator and gamma ray detectors will have to be raised on movable scaffolds.

If the necessary funding is raised, the lost painting could be found thanks to science—which Leonardo, of all painters, would probably appreciate most. ✪

Funding for the project has been provided by the National Geographic Society.



Painting is poetry which is seen and not heard, and poetry is a painting which is heard but not seen.
— Leonardo da Vinci

A lost Leonardo da Vinci masterpiece may lie hidden behind this fresco in Florence's "Hall of 500." Photo courtesy Dave Yoder/National Geographic Society.



THE MINIMAL

by Jen Salazar and Christopher Henry

MICROBE

How many genes can you strip from a cell and still call it a cell?

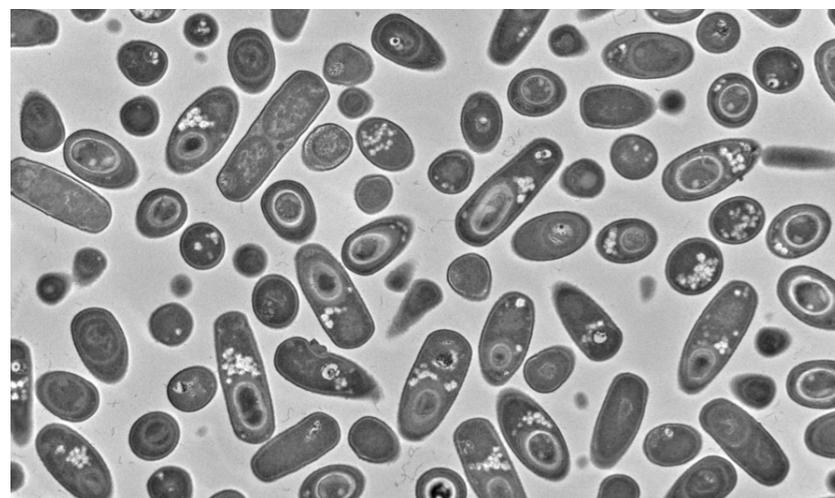
There are approximately one trillion quintillion microbial cells on this planet. That's more than the number of stars in the known universe!

Microbes are not only numerous but also incredibly diverse, occupying extreme habitats where little else can survive—down a thermal vent in the deep ocean or bathing in a pool of near-boiling hot acid. They also perform a wide range of useful functions, such as reducing uranium to remove it from groundwater and degrading complex polysaccharides so we can digest our food.

Microbes are humanity's secret companions, playing silent but starring roles in global biogeochemical cycles, animal and human diseases, fuel production, bioremediation, food chains, and agriculture. Many microbes dwell inside each of us. We are beginning to understand that microbes don't merely inhabit our guts to aid digestion; they have co-evolved in a symbiotic relationship with us. Gut microbes are now known to affect brain development, immune and liver functions, and adult behavior.

To study these microbes and the complex communities they form in the environment, Argonne and

three other national laboratories (Lawrence Berkeley, Brookhaven, and Oak Ridge) are collaborating to build a research tool called the Systems Biology Knowledgebase, or "KBase." Systems biology studies complex interactions in biological systems, such as the enzymes in a metabolic pathway. Studying these interactions involves vast amounts of interrelated data of



different types. Currently, this data can't be easily combined; it exists in different formats in unlinked databases associated with different research tools. KBase aims to change this, but its goal is larger than data integration. The team seeks to advance research in two broad, important areas: plants and microbes.

Microbial research underlies many interesting areas of work at Argonne. Some studies search for useful

functions that might be harnessed for human benefit; others focus on identifying the biological machines that drive the life processes of an individual cell, with the eventual goal of rewiring the cell to perform a useful task.

Biologists often learn by eliminating a portion of the cellular machinery and observing how that machinery responds. Argonne takes

this approach to the extreme with an effort to synthesize a "minimal cell"—a cell containing only the biological machines that are essential for survival.

The first step is to compile what we actually know about the genomes of existing microbes. Argonne, the Fellowship for Interpretation of Genomes, and the University of Chicago developed and maintain a database that is part of a resource called The SEED, which collects all

known functions of different genes. Scientists use another tool called ModelSEED to show how genes and proteins with known functions interact to carry out all of the tasks that a cell must perform. Then they use the model to speculate on what is missing and to fill in the gaps, applying knowledge of evolutionary relationships to assign likely functions onto unlabeled genes.

Researchers also need to conduct lab work to verify the work done "in silico" (on the computer). Argonne scientists begin with a real microbe found in nature; in this case *Bacillus subtilis*, a common soil bacterium. Through trial and error, they knock out different genes and check whether the cell can still grow in a petri dish. If a microbe grows despite the mutation, they can label that gene as not vital for survival.

This is a simple approach, but it can get very complicated in execution. Imagine a car. If Argonne scientists applied their method of cell studies to understanding exactly how a car works, they would first try to build a "minimal car," and add extra features later.

They would begin with a whole fully featured, functioning car, then randomly remove a part and determine whether the car still functioned. If the removed part didn't keep the car from running and transporting passengers, then the scientists would say that part is not essential. When possible, they would record the role that part performed,

and continue at random until every single car part has been removed and tested.

But as one might guess, this technique is not always straightforward. Some parts interact with or preclude each other. Some parts are at least partially redundant. For example, what if you only remove one tire? The car might still move, though admittedly not very well. But if you take away the axle rod, even if the tires are perfectly intact, the car won't be able to move. Genes are frequently interconnected in this way too, so researchers must keep track of their dependencies and interactions.



The environment also matters. When you strip the car down to its most basic version, the result might not be a very robust vehicle. The number of features that you can strip off depends on where it is intended to travel. For example, do you only need the car to run on a very smooth and flat road? If so, you can probably safely toss a lot of inessential parts. But if you're expecting to drive uphill over obstacles, you may not want to toss the shock absorbers.

Likewise, the environment of a cell matters. You can take more out

Electron microscopes capture *Bacillus subtilis* bacteria. Images courtesy Kumaran Ramamurthi, National Cancer Institute.

of a cell if it's destined for a friendly environment already supplied with nutrients in a ready-to-go form. But a cell placed in a nutrient-poor petri dish will need some metabolic equipment to be able to feed itself.

Breaking the cell down to the minimum components necessary and unraveling the interplay between genes, pathways, and proteins and phenotype is essential for understanding how cells work, being able to model cells, and eventually reengineering cells to help solve critical problems.

The more we find our lives linked to those of the diverse microbes around us, the more vital it becomes to understand them.

Constructing a minimal cell and sharing that data across the scientific community will accelerate solutions for everything from energy to human and animal diseases. By integrating and analyzing this kind of data, KBase will enable researchers to design and interpret their experiments more powerfully, and to quickly share those results and their interpretations. In the future, new functions will let users visualize data, create models, and design experiments based on KBase suggestions to target the most critical work. 

This work was supported by the Department of Energy's Office of Science.



a natural solution for transportation

by Jared Sagoff

As the United States transitions away from a primarily petroleum-based transportation industry, a number of different alternative fuel sources—ethanol, biodiesel, electricity, and hydrogen—have each shown their own promise. Hoping to expand the pool even further, Argonne researchers have begun to investigate adding one more contender to the list of possible energy sources for light-duty cars and trucks: compressed natural gas (CNG).

Compressed natural gas is composed primarily of methane, which when compressed occupies less than 1% of the volume it occupies at standard pressure. CNG is usually stored in cylindrical tanks that would be carried onboard the vehicles it fuels.

Because the domestic production of natural gas has increased dramatically over the past ten years, making a large number of the cars and light trucks currently on the road CNG-compatible would help improve U.S. energy security. “As a country, we don’t lack for natural gas deposits,” said Argonne mechanical engineer Thomas Wallner. “And there are fewer obvious challenges with direct supply than with most other fuels.”

Natural gas currently comes primarily from deep underground rock structures, including shale.

Recent improvements with hydraulic fracturing, or “fracking,” a controversial process that some critics claim can hurt the environment, have made it economical for natural gas companies to extract a greater supply of natural gas from unconventional sources.

Like gasoline, both the production and combustion of CNG release greenhouse gases into the atmosphere. To be able to make an accurate comparison to gasoline, scientists and engineers will need to look at each stage of the fuel’s production and use, said Argonne environmental scientist Andrew Burnham.

Unlike gasoline, however, CNG markets are relatively insulated from geopolitical shocks, said Wallner.

“The price of CNG has been and will probably continue to be both cheaper and more stable over the long term than gasoline,” he said.

CNG currently costs the equivalent of about \$2 per gallon, roughly half that of current gasoline prices, according to Wallner.

In order for CNG to take hold, many more stations will need to offer it as an option, and the infrastructure for delivering and distributing the fuel around the country will have to be built up. There are currently fewer than 1,000 publically available CNG refueling stations in the United States, in comparison to nearly 200,000 gas stations.

Argonne already has the capability to help automotive industry leaders test and analyze CNG vehicles. In particular, Argonne’s Greenhouse

Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model gives experts the ability to examine the greenhouse gas emissions of various fuels from “well-to-wheels,” involving each stage of production, distribution, and combustion. “We have years of expertise working with industry to develop alternative-fuel vehicles as well as the tools necessary for the public to understand the impact of these vehicles on the environment,” said Argonne mechanical engineer Michael Duoba.

Although CNG vehicles emit fewer greenhouse gases than conventional automobiles as fuel is combusted, “upstream” challenges in production and distribution of CNG—particularly methane leakage—make it somewhat less attractive when it comes to preventing climate change. “There are a lot of points in the lifecycle of the fuel where we still need better data,” Burnham said. “There are technological opportunities for us to capture the leaked natural gas and reduce greenhouse gas impacts.”

For heavy-duty applications, like city buses, CNG might have the potential to cut down emissions of particulate matter and nitrogen oxides, helping municipalities meet more stringent EPA standards enacted in the past few years, according to Burnham.

In Wallner’s view, CNG vehicles—like plug-ins and diesel-powered automobiles—will serve the transportation needs of some, not all.



“It’s important to see each of these technologies as a part of the solution but not the entire solution,” Wallner said. **“The more we invest in their development, the closer we’ll come to a portfolio that makes sense both economically and environmentally.”** ❄️

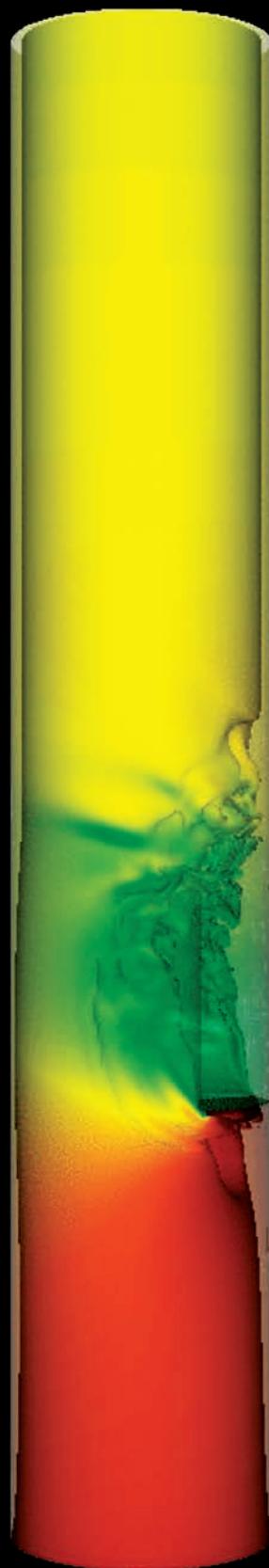
Argonne engineer Thomas Wallner is part of a group working to analyze compressed natural gas as a fuel.

This research is supported by the Department of Energy’s Office of Energy Efficiency and Renewable Energy.



SHARP could shave millions off nuclear reactor design costs

by Renee Nault



This simulation shows a coolant channel that has been partially blocked. Predicting how coolant behaves in unexpected situations helps enhance safety and reactor performance. Image courtesy Paul Fischer and the SHARP thermal fluids team.

Back in the earliest days of nuclear energy, Argonne physicists and engineers used slide rules and their own basic knowledge of reactions and physics to design nuclear power plants. Then, beginning in the early 1960s, they enlisted computers to develop designs with data from experiments and actual reactor testing. Over this entire span, Argonne built more than 85 experimental reactors to test its reactor designs and computer programs—each a costly and time-consuming endeavor.

Despite all this, many of the highly complex physical phenomena that affect reactor performance and safety remained somewhat of a mystery. It wasn't possible to “see” what was taking place inside this very harsh environment—until now.

Researchers are using some of the world's most powerful computers at the Argonne Leadership Computing Facility to take a leap forward in nuclear reactor design, analysis, and engineering. Their efforts could shave millions of dollars off the cost of reactor design, development, preparation for licensing, and construction.

Researchers have developed a suite of computer tools, called the

Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) Reactor Performance and Safety Simulation Suite, which numerically mimics and allows researchers to “see” the physical processes that occur in a nuclear reactor core. SHARP users can build complex virtual reactor models to run the reactor through a variety of operational or accident scenarios that would be impractical or impossible in the real world.

SHARP builds upon existing computer codes used to conduct safety evaluations of today's aging nuclear reactors. When you want to use those older codes to virtually test new reactors, however, you run into a few problems. They're well-calibrated for evaluating the safety of new reactor designs, but aren't so great for optimizing designs for efficiency or cost. SHARP has been written specifically to simultaneously

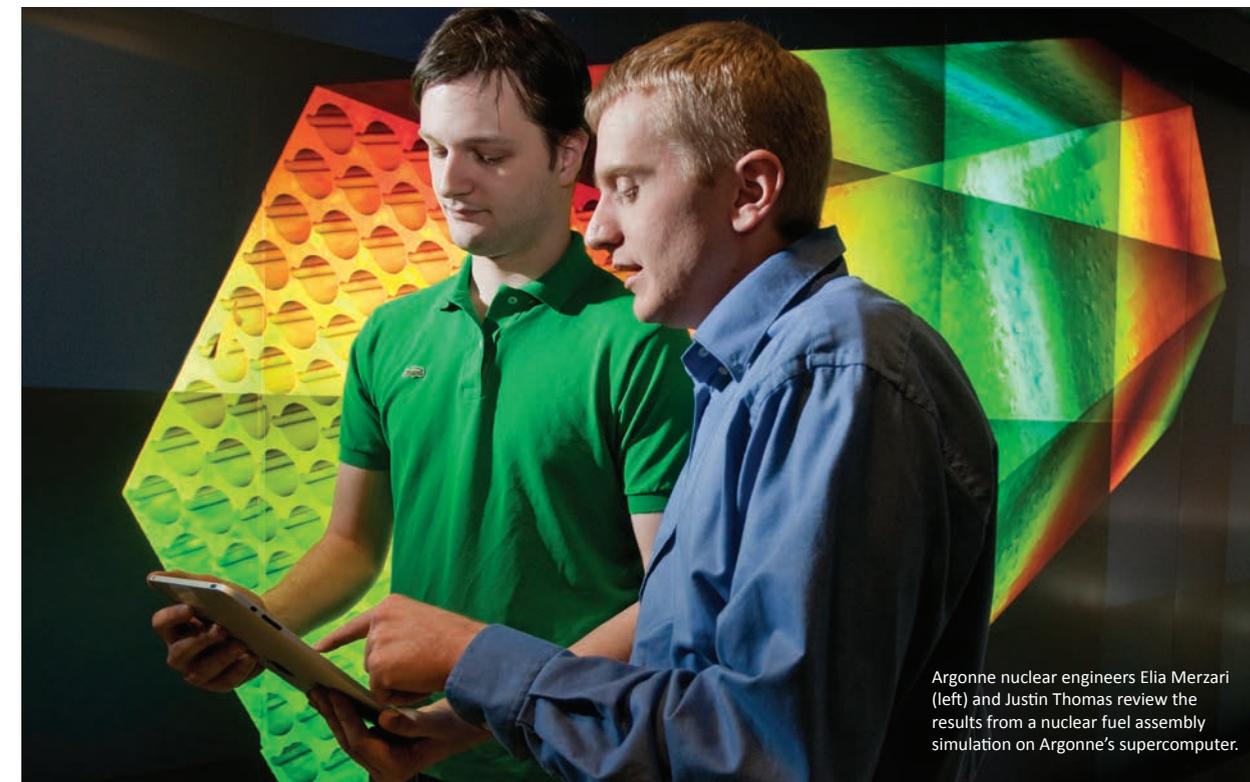
look at the safety, lifetime, and performance of different advanced design ideas.

Idaho National Laboratory, Lawrence Livermore Laboratory, Oak Ridge National Laboratory, and other U.S. DOE and university collaborators have also contributed to SHARP.

This is a perfect fit for Argonne's nuclear program, which has half a century of experience with reactors under its belt and one of the world's

largest concentrations of researchers involved in advanced reactor design. For example, early in the program, the code creators wanted to test how accurate the codes could be. They built a virtual model of one of Argonne's historical test reactors, the Zero Power Reactor, ran “experiments” on it, and checked how well the computer results matched up against the actual data.

Modern codes like SHARP are already successfully replacing some types of nuclear experiments. SHARP's next step is refining the code to make it run more efficiently on powerful supercomputers like Argonne's new Blue Gene/Q (see page 26). More efficient codes mean scientists can run more tests during the same computer time with fewer problems, making SHARP a more useful tool for reactor designers around the world. ☼

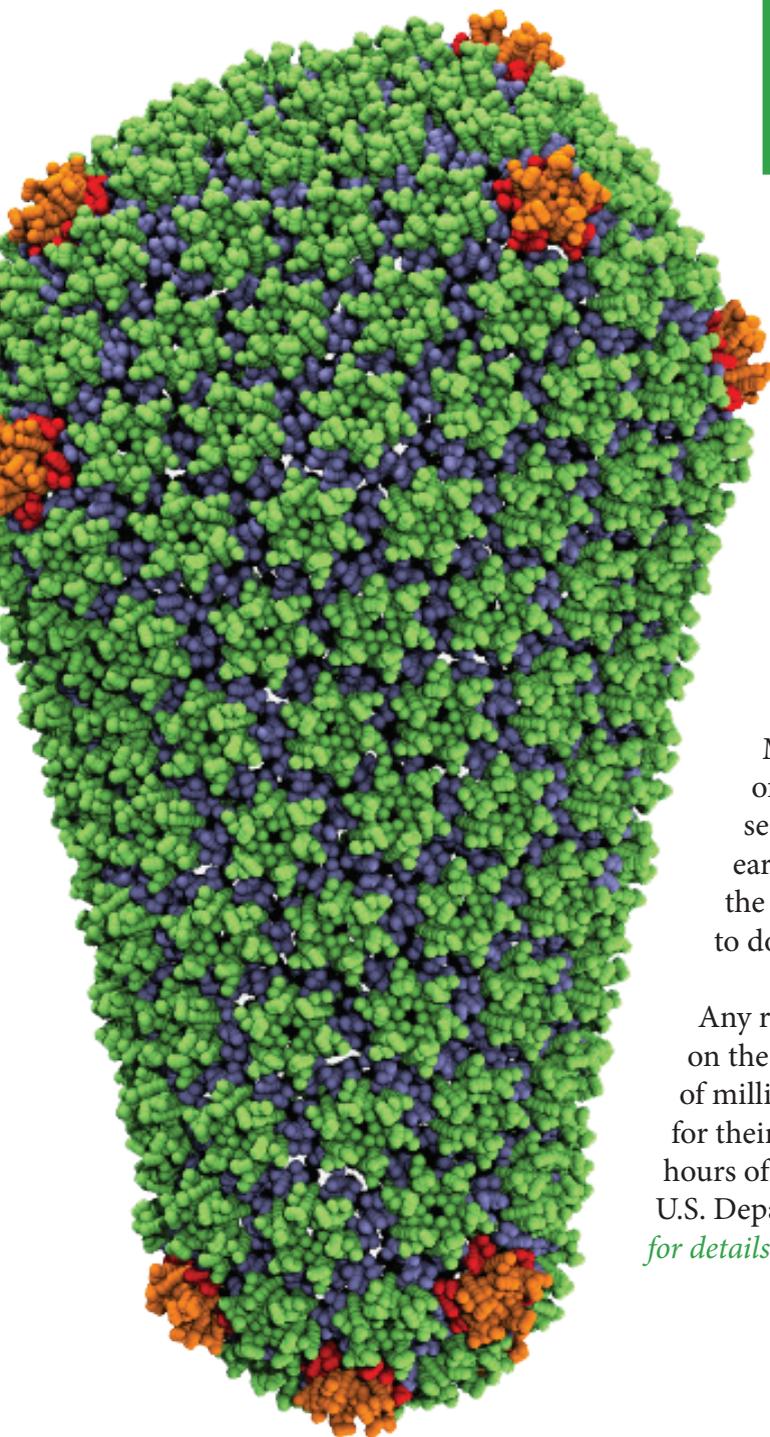


Argonne nuclear engineers Elia Merzari (left) and Justin Thomas review the results from a nuclear fuel assembly simulation on Argonne's supercomputer.

SHARP is funded by the Department of Energy's Office of Nuclear Engineering, Advanced Modeling and Simulation Office, and the Nuclear Energy Advanced Modeling and Simulation Program.

INTRODUCING MIRA

by Louise Lerner



Argonne's new supercomputer won't be in full production until 2013, but it represents such a leap forward that just the first two prototype racks already rank among the top 100 fastest computers in the world.

The computer, named "Mira," is an IBM Blue Gene/Q, the third generation in a line of supercomputers that has topped the performance charts. Argonne and its sister national lab Lawrence Livermore helped design the computer, which will be the third fastest supercomputer in the world.

Mira will be a 10-petaflop machine, capable of carrying out 10 quadrillion calculations per second. If you recruited every single person on earth to solve one calculation per second, around the clock, it would take them more than two weeks to do the work that Mira will do in one second.

Any researcher with a question can apply for time on the supercomputer, typically in chunks of millions of processor-hours, to run programs for their experiments. This adds up to billions of hours of computing time, awarded through several U.S. Department of Energy programs; [see page 31 for details.](#)

"BILLIONS OF HOURS?" Time on the supercomputer is measured in processor-hours, or the work done by one processor in one hour. Since Mira has almost 800,000 processors, that adds up quickly.

Scientists will use Mira to study exploding stars, nuclear energy, climate change, and jet engines, to name just a few projects—see the sidebar on page 31 for more.

Beyond providing hours of computing time, Mira itself is a stepping stone toward the next great goal of supercomputing: exascale speed, where computers will calculate quintillions of floating point operations (or "flops") per second. That's a thousand times faster than today's top machines.

What does a supercomputer need to be the best?

SPEED

Mira will be 20 times faster than Intrepid, its predecessor at Argonne. It will provide billions more processor-hours per year to the scientists, engineers, and researchers who use it to run complex simulations of everything from nuclear reactors to blood vessels.

The first supercomputers consisted

of a handful of processors and memory units that were much faster than mainstream computers. As demand for ever-faster computers grew, and microprocessors got cheaper, the industry began instead combining hundreds—and then thousands—of processors, or "cores," into one system. Argonne's current supercomputer, Intrepid, has 163,840 cores; Mira will have 786,432. (A typical laptop has two cores.)

"Each individual core in the Blue Gene architecture is actually slightly less powerful than the ones found in a typical home desktop computer," said Michael Papka, who heads the Argonne Leadership Computing Facility. "But because faster processors generate more heat, at the petaflops level it's more efficient to run lots of lower-power processors."

Mira's sister machine, a Blue Gene/Q destined for Lawrence Livermore National Laboratory, will run at 20 petaflops. It will be the fastest supercomputer in the world—the first time since 2009 that a U.S. supercomputer will top the list.

EFFICIENCY

Mira is expected to be the greenest supercomputer in the world, topping supercomputing's Green 500 list even before it's installed. It's five times as energy-efficient as its predecessor.

It has to be: "If you took the current Blue Gene supercomputer and simply added processors to get it to exascale speed, which is 2,000 times faster than today's machine, you'd need a couple of new power plants just to supply electricity to it," said Pete Beckman, who heads Argonne's exascale initiative. Each new computer has to break new ground for efficiency just to keep up.

Mira's predecessor Intrepid, itself a revolutionary energy saver when

it was built, uses chilled water to cool air that is circulated around the processors. In Mira, copper tubes will pipe cold water directly alongside the chips, which saves power by eliminating the extra cooling step.

Mira also fits more cores onto a single chip. This arrangement reduces the distance that data has to travel between the chips, which speeds communication between cores and saves the energy lost when transporting data across long distances. > > > *continued*

NUMBER-CRUNCHING

3rd fastest supercomputer in the world

5 times more energy-efficient than its predecessor

20 times faster than its predecessor

10 petaflops

48 separate racks

96 tons

786,432 processors

5+ billion computing hours allotted to scientists every year

10 quadrillion floating-point operations per second

FAULT TOLERANCE

“Any complex system designed by humans must anticipate breaking down,” Beckman said. “And since these supercomputers have many, many cores, there are many, many spots for something to go wrong.”

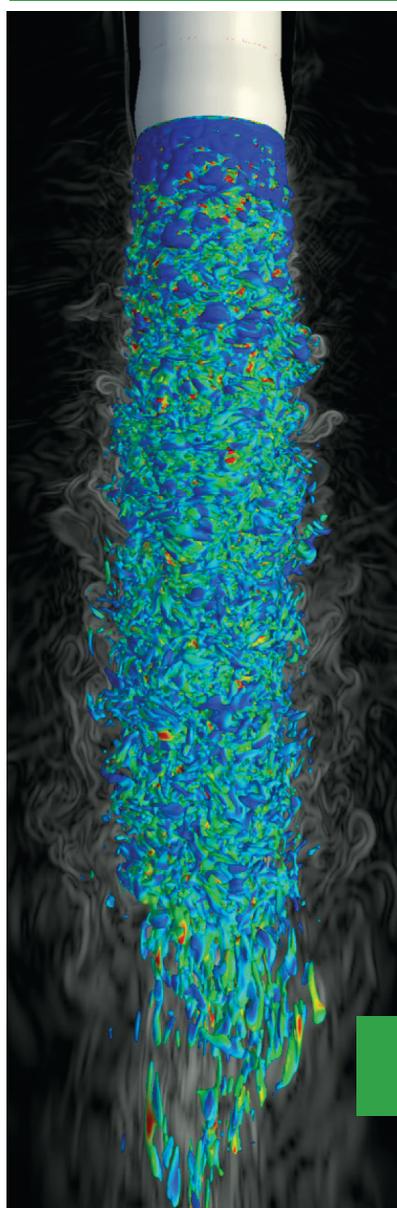
One or two misbehaving cores can halt the entire task, Beckman said, because most codes are designed to be interdependent: each core gets a task and they feed the results to one another. If one goes down, the rest of the operation gets hung up while waiting for the missing answer. Because a supercomputer’s system is so complex, designing it to crash less often—and to wreak less havoc when it does—is a delicate art.

There are several ways to make a computer more resilient; for example, reducing the number of parts. “Every time you’ve got a connector, you’ve got a potential for failure,” Papka explained. Mira’s memory chips and CPUs are soldered directly onto cards.

Another technique saves wear on data storage. As the computer works, it’s constantly saving, erasing, and rewriting data. Over time, this wears out the chips. One way to fight this is “wear leveling”: writing software that moves the storage location around the card to distribute the wear equally. It’s a bit like rotating tires on a car.

Argonne’s previous Blue Gene/P system was designed to go five to six days without error. In fact, the computer has consistently outperformed that hope—it often runs for weeks without crashing. Mira is predicted to be stable enough to run without crashing for up to 10 days, even though it has 623,000 more cores than Intrepid. Experts say that fault tolerance will become even more crucial as computers get closer and closer to exascale speeds.

The name “Mira” comes from the Latin for *wonderful, surprising, remarkable, extraordinary*. It’s also similar to the Italian word *mirino*, which means *viewfinder*. Both refer to the discoveries Mira will enable once the machine is fully up and running.



USER FRIENDLINESS

Though some of Mira’s architecture is different, it is also grown from the same DNA as its predecessor at Argonne. For programming purposes, it’s very similar—only much faster.

“Users will be able to run the same codes on Mira as they did on its predecessor,” Papka said. “They will be able to jump straight into running their scientific programs without having to rewrite their codes from scratch.”

For the problems that do pop up, the Argonne Leadership Computing Facility, which runs the supercomputer, has a crack team to help users adapt their codes and fix unexpected bugs.

Solving Problems with Supercomputers

Mira’s numbers are impressive, but why do we need supercomputers in the first place?

“Supercomputers help the United States economy stay ahead of our competitors,” Beckman said. These days, more and more companies rely on modeling and simulation.

Take planes. “Say that an aerospace company wants to build a new airplane,” Beckman said. “In the old days, they’d have to physically build models of all the wing types they were considering and test them all in wind tunnels. Today, they can run a very detailed simulation and virtually test the air flow in hundreds of models before building just a few physical versions, which saves a lot of money and time.”

The oil and gas industries are also investing in computation. Plugging geologic models into computers creates maps that lead companies to the right places to drill, reducing the environmental and financial costs of drilling unnecessary wells.

Simulation of noise from jet exhaust nozzles. Data from General Electric Research, visualization by Joe Insley (Argonne).

That virtual design space is useful for more than consumer products and drilling. It’s also key to studying climate change.

The world’s climate is an extraordinarily complicated affair. It sews together temperature, cloud cover, vegetation, rainfall, wind, geography, ocean currents, even volcanic eruptions, all over the nearly 200 million square miles of Earth’s surface area.

Even today’s most accurate climate models use just a single data point to represent thousands of square miles. An area the size of Lake Michigan is represented by perhaps two data points, which can’t possibly convey the rich interplay of lake, dunes, forests, swamps, and farmland—not to mention the sprawling urban heat island of Chicago—in enough detail to make accurate predictions. More powerful computers allow scientists to incorporate more and more data to create higher-resolution models.

With Mira, scientists will also be able to run their models faster and more often. More runs allow the scientists to test how much the model changes depending on what data goes into it, which gauges uncertainty. When meteorologists predict the week’s weather for Chicago, they run the current weather data through different

models dozens of times. Do all of the models agree on two inches of snow by Friday, or do some say two inches and some say two feet? The more times they run a model, the better they can estimate just how uncertain they are about the forecast. Similarly, climate scientists can both improve their models and better understand how accurate their models are.

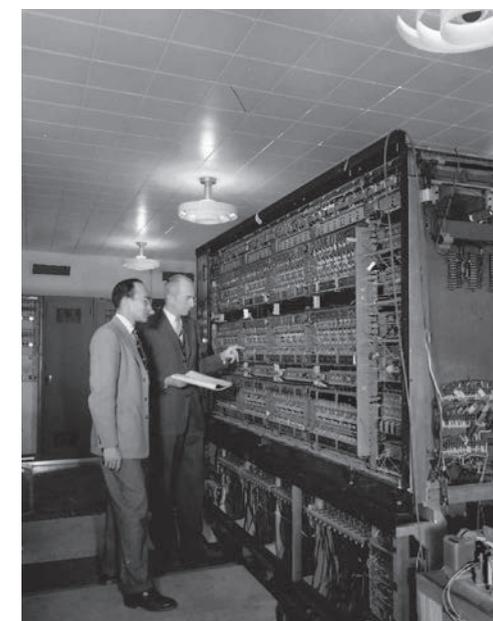
Finally, improvements in supercomputers tend to trickle down into the consumer’s hands. For example, all supercomputers depend on parallel processing: breaking a task into many smaller ones that

can be performed simultaneously. Today, almost all laptops, PCs, and smartphones run on this principle, dividing tasks between two cores.

The research and planning that go into the next generation of supercomputers like Mira help advance the field of computer science, making computers faster and more energy-efficient.

But for the hundreds of scientists who will use it to tackle some of the biggest scientific questions in the world, Mira’s contribution is just beginning.

Mira is supported by the Department of Energy’s Office of Science, Office of Advanced Scientific Computing Research.



THEN

AVIDAC was Argonne’s first digital computer. Designed and built by Argonne’s Physics Division for \$250,000, it began operations Jan. 28, 1953.

“If you have an iPhone, you’re carrying a computer in your pocket that is far more sophisticated and powerful than the first supercomputer we built at Argonne back in 1953.”

— Argonne computer scientist Charlie Catlett

THE ALCF

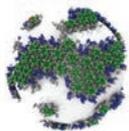
Mira is the latest resource in the DOE’s Office of Science user facility that is managed by the Argonne Leadership Computing Facility (ALCF), one of two DOE leadership computing facilities in the nation. When scientists from around the world come to Argonne to run their programs on Mira, ALCF staff help adjust their codes to get the best performance out of the supercomputer. Supercomputers are very different from your average university computing cluster, and a program written for the cluster won’t take full advantage of Mira.

NOW

Mira is the third fastest supercomputer in the world.



alcf.anl.gov



Fifteen Minutes with Rick Stevens

by Vic Comello

Argonne Now's Vic Comello asks associate lab director Rick Stevens about the next leap in supercomputing, what needs to happen before we get there, and what it will help us do.



Rick Stevens

VC: In what ways will exascale computing transform the world?

Stevens: Every time we have more computer capability, we come up with new ways of doing things, and the most interesting things that we tend to do on the big machines are not the things that we thought we would do initially.

For example, when the current parallel computers were designed years ago, the field of genomics was still in its early stages. Now one of their most significant uses is to assemble and analyze genomes. Massive studies comparing genetic variability across thousands of people to look for disease correlations was an area that we didn't even imagine possible, say, 10 years ago.

So when we talk about machines 10 years from now, my sense is that even if I came up with compelling examples right now, they wouldn't be the things that actually transform the world, because those are going to be the things that we haven't thought of yet that will suddenly become possible when the machines exist.

VC: What kinds of applications can be foreseen?

Stevens: Almost every area of science has problems that are not solvable or not even approachable on the current generation of computers. With an exascale machine, for example, we will be able to simulate neural networks of the complexity of the human brain. We should also be able to design microorganisms for specific applications; for manufacturing biofuels, say, or synthesizing interesting or valuable chemicals such as vitamins or drugs.

These machines will offer incredible design capabilities, whether you are designing climate models or nuclear reactors or even skyscrapers, partly because you can not only perform huge simulations but also do many

computational experiments simultaneously in which you vary the parameters of your models. Rather than seeing one answer, you would see a whole bracketing of possible results, yielding error bars that say there is a 90% probability that the system will operate in this range and a 50% probability it'll be in that range, and so on. That capability appeals to design engineers because they want to have confidence in their projections.

VC: What problems do we have to address before we get to exascale?

Stevens: Reliability is one area that must get addressed. Say you have a machine today with 1 million processors that stays running for 10 days before something goes wrong; thus 10 days would be its mean time to failure. Now let's say we have an exascale machine that is 1,000 times bigger. If we used the same technology in making the machine, it would go down 100 times per day, because its failure rate per element would be the same. That means in order for these exascale machines to actually be useful, they would have to become a lot more reliable.

We will probably have to find another factor of 10 or 100 in reliability in order for the machine to be as reliable as current machines are. Some of the increased reliability might come from hardware, but when you're writing a program for one of these machines, you might have to specify what parts of your data need to be preserved when the machine goes down and what parts you can recreate after a failure. Biological systems do this sort of thing all the time. Cells in your body are being replaced all the time, and you don't even notice. We don't yet have that capability with these machines, in which individual processing units fail and are replaced while the machine keeps going, but it is certainly a goal.

DID YOU KNOW?
IBM Blue Gene computers have helped chessmasters train for the World Chess Championships.



alcf.anl.gov/mira
search | argonne mira

Prepping Mira for Showtime

by Cheryl Drugan

To hit the ground running with Mira, the ALCF staff is working with 16 research teams from across the nation to test their codes on Blue Gene/Q prototype hardware. This period helps catch system bugs and instabilities before Mira goes into full production.

The 16 Early Science Program projects have more than two million core hours allocated to them. Here are just a few:

WATCH A STAR EXPLODE

White dwarf stars explode in thermonuclear-powered explosions called Type Ia supernovae. Scientists think that a process called turbulent nuclear combustion sets the stage for a detonation that incinerates the star, causing it to explode (see images at right). Astrophysicist Donald Lamb (University of Chicago) is investigating by creating simulations of turbulent nuclear combustion.

THE BEST AIRPLANE WING

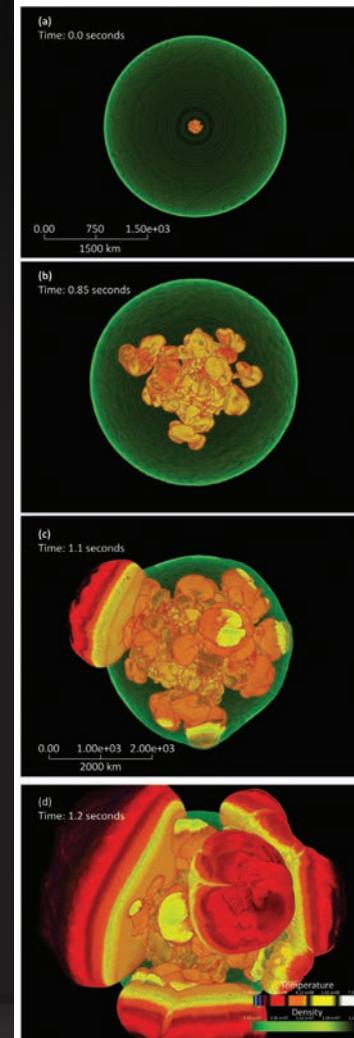
Another project simulates the airflow across aircraft and wind turbine blades. Kenneth Jansen (University of Colorado-Boulder) is testing small attachable devices, called "synthetic actuators," that can tweak the cross-surface airflow to increase efficiency and reduce damage to airplane wings.

A CATALYST FOR CHANGE

Argonne materials scientist Larry Curtiss is running simulations of electronic structures to find new materials for electrical energy storage and catalysis. New catalysts are a key component of making biofuels cheaper and more efficient. (More about Curtiss's work is on page 42).

THE SKELETONS OF CELLS

Our cells are built on sturdy frameworks using proteins called "microtubules." Despite their importance, there's a lot we still don't know about them. Gregory Voth (Argonne, University of Chicago) studies the physics that happen on a molecular level to let microtubules work their magic.



Four snapshots of a simulated star as it explodes. Image by Donald Lamb.



Panagiotis Prezas examines a battery cell in Argonne's Electrochemical Analysis and Diagnostics Lab, where scientists test batteries' life cycles and calendar lives.

Imagine if you only had to plug in your phone once a week. Or your laptop lasted days between charges. Or an affordable electric car that ran for more than 300 miles on a single battery charge.

That wonderful battery is still a gleam in the eyes of scientists working in Argonne's energy storage program, but their work is bringing that dream closer all the time.

Last year, more than a decade's worth of battery research and development at Argonne made its way into the world's first mass-produced plug-in hybrid electric car: GM's Chevy Volt. Argonne's material helps the battery—a lithium-ion design similar to those in your cell phone or laptop—last longer, run more safely, and perform better at lower cost than other batteries currently on the market.

As demand grows for electric and hybrid cars, automakers are searching for the battery that will make those cars compete with gasoline. Almost fifteen years ago, GM's short-lived EV1, star of *Who Killed the Electric Car?*, ran on a battery that weighed 1,175 pounds. The battery in the hybrid Volt weighs in at a svelte 435 pounds.

But the next generation of batteries, according to Argonne materials scientist Khalil Amine, will be 50% more energetic—so automakers could double the range or significantly drop the price and size of the battery. We'll need a battery like this to make electric cars available to anyone who wants to buy one.

Lithium-ion is a relative newcomer to the battery scene: it wasn't until 1991 that the first commercial Li-ion batteries went into electronics. They're ideal for cars because they pack a bigger punch per ounce than any other kind of battery currently on the market.

What exactly happens inside Li-ion batteries? They are named for lithium ions, which shuttle back and forth between the two poles of the battery. When you charge a battery, you are using electric current from the outlet to drive all of the lithium ions over to one pole, called the anode. As soon as you unplug the battery and begin to use it, the lithium ions flow back to the cathode,

which generates a current that powers your laptop.

About the same time that the EV1 hit roads, Argonne researchers Chris Johnson and Michael Thackeray set out to improve lithium-ion cathodes even further. Early commercial Li-ion batteries were still new and expensive, somewhat unstable when fully charged, and just couldn't make the cut for a cheap all-electric car.

The scientists wanted to find a material to stabilize the battery that would also be cheap and safe—essential if you want to manufacture batteries for millions of cars and laptops.

In the cathode, atoms sit side by side in rows. When lithium ions are pulled out of the cathode during charging, they leave holes behind in the structure. The more lithium ions that can circulate during charge and discharge, the better the performance, but too many holes and you run the risk of ruining the structure.

“We tackled the problem in a unique fashion,” Thackeray said. **“Our idea was to embed a sort of ‘skeleton’ into the cathode. It’s inactive, but it serves as bones that help keep the structure intact when lithium ions are pulled out.”**

The Department of Energy's Office of Basic Energy Sciences funded early research; later support came from DOE's Office of Energy Efficiency and Renewable Energy.

The resulting integrated structure is highly complex. “It's very difficult to determine exactly how the atoms are arranged at the molecular level,” Thackeray said. “If we understand the routes that lithium ions take as they move in and out of the structure, and the damage that occurs when this happens, it will allow us to think of ways to stabilize the structure.”

> > > *continued*

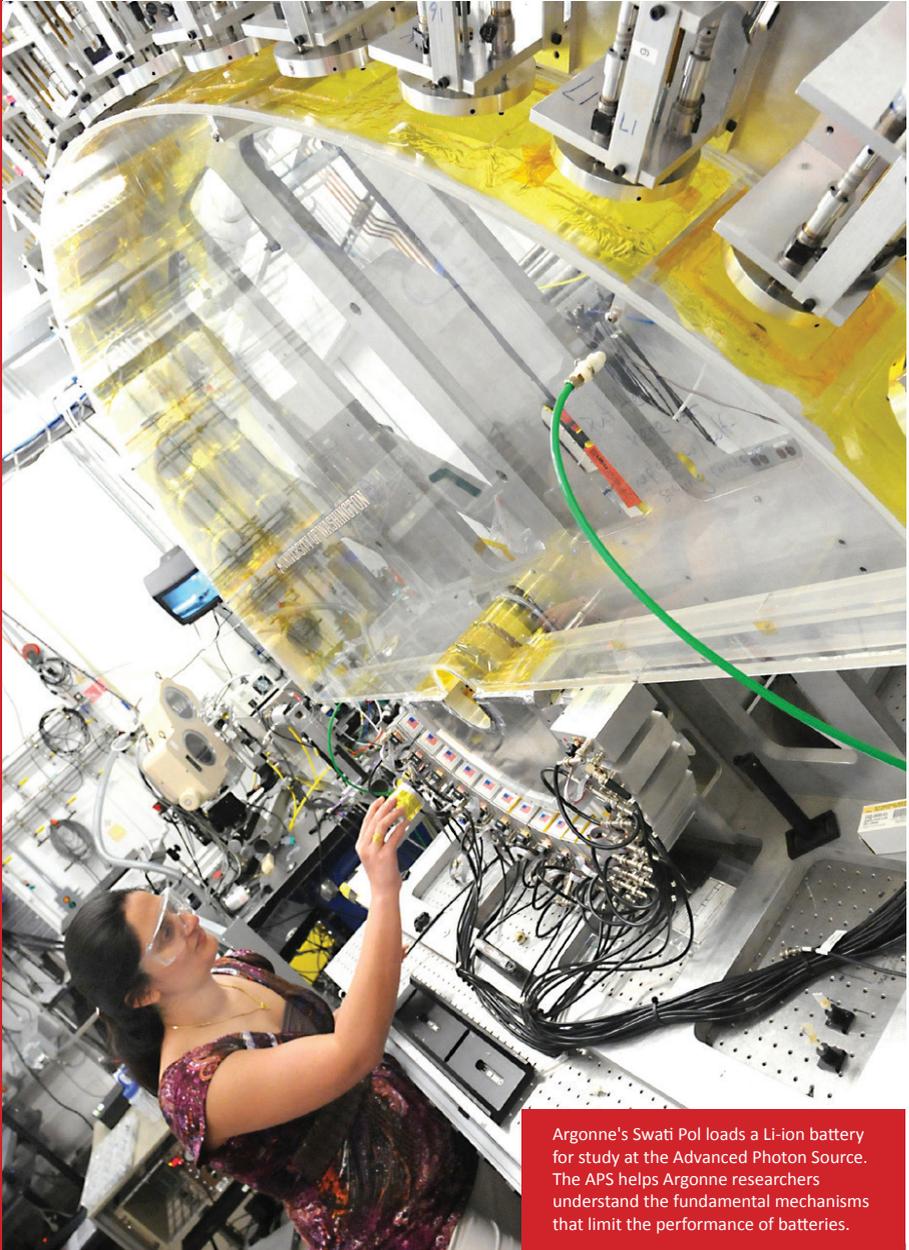
by Louise Lerner

THE SEARCH FOR A

SUPERBATTERY

How Research at Argonne will Help Power the **Next Generation** of Electric Vehicles

Argonne researcher Sabine Gallagher prepares a surface area analyzer for characterizing battery materials.



Argonne's Swati Pol loads a Li-ion battery for study at the Advanced Photon Source. The APS helps Argonne researchers understand the fundamental mechanisms that limit the performance of batteries.

“Having these large facilities like the Advanced Photon Source helps us enormously to characterize the battery materials.” – Michael Thackeray, Argonne battery scientist

But it's one thing to make a tiny sample for a lab test and another to make that process work consistently at the huge scales required for factories to make cheap batteries. This was Khalil Amine's challenge: improve the synthesis process. "When you're manufacturing a battery, the way you synthesize it is absolutely key to how good the battery actually is," Amine said. "You have to get the exact right temperature, starting chemicals, reaction times, and environment—all the parameters have to be right." He set up a lab to focus on identifying reactor processes to turn out materials more consistently. When battery companies became interested in the technology, they sent their staff to Argonne to learn how to make the materials.



THE NEXT HORIZON

Amine, Thackeray, and others are already working on the next generation of Li-ion batteries. They are close to making significant advances. The next generation will allow more lithium to cycle freely through the battery, which will significantly boost the battery's capacity—but there are still a few bugs to work out. "Advances come in cycles," Amine said. "We find a

problem, we fix it, we find another problem, we fix that problem too." Amine thinks this new generation will be a vast improvement on the last one. "We're looking at increasing the energy by another 50%," he said. "That means a huge reduction in the cost of the battery or a huge jump in how far you can go on a single charge." But even the most perfect Li-ion battery wouldn't be quite on a par with gasoline, which is one of the most energy-dense substances on Earth.

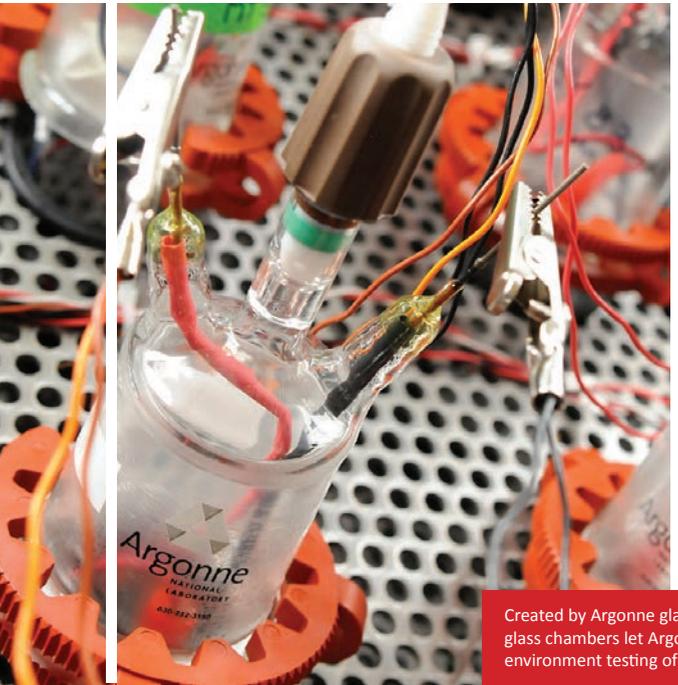
one that pulls close to gasoline. It could take that imaginary electric car 500 miles on a single charge. Right now, though, Li-oxygen technology has a lot of problems. For one, Li-oxygen batteries don't recharge efficiently. What we need is a good catalyst to help make and break the lithium and oxygen bonds more easily. (For more about catalysts, turn to page 42). To tackle the challenge, Amine, Thackeray and their teams are partnering up with scientists across Argonne and calling in the big guns—the Advanced Photon Source and Blue Gene supercomputer, Mira—to help them solve the materials problems posed by lithium-oxygen batteries.

The Advanced Photon Source, Argonne's large X-ray synchrotron, helped shine a light on the matter. Johnson paired with scientists who specialize in spectroscopy to use brilliant X-rays to come up with a picture of the materials at the atomic level. "We can even put the materials in a whole working battery and watch what happens while the battery cycles," Johnson said.

To find the best mixture for the cathode, the team tested dozens of combinations—first creating the new materials, then checking performance in actual batteries. They also upped the charging voltage to 4.6 volts—considerably higher than the usual—and saw the cathode's capacity double.

“Seeing homegrown innovations going into a large-scale production car that's helping electrify the American fleet—that's really exciting and good for the country. It's really the ultimate goal for a researcher.”

—Chris Johnson, Argonne battery chemist



Created by Argonne glassblower Joe Gregar, these unique glass chambers let Argonne researchers conduct controlled environment testing of lithium-oxygen batteries.

For now, though, the next big breakthrough might be just around the corner. "In science, you never really know quite how things are going to play out," Thackeray said. "There's an element of intuition, of knowing the direction you want to take, and a bit of luck. It's a very exciting time to be a battery researcher." ❁

BATTERIES FOR AMERICA

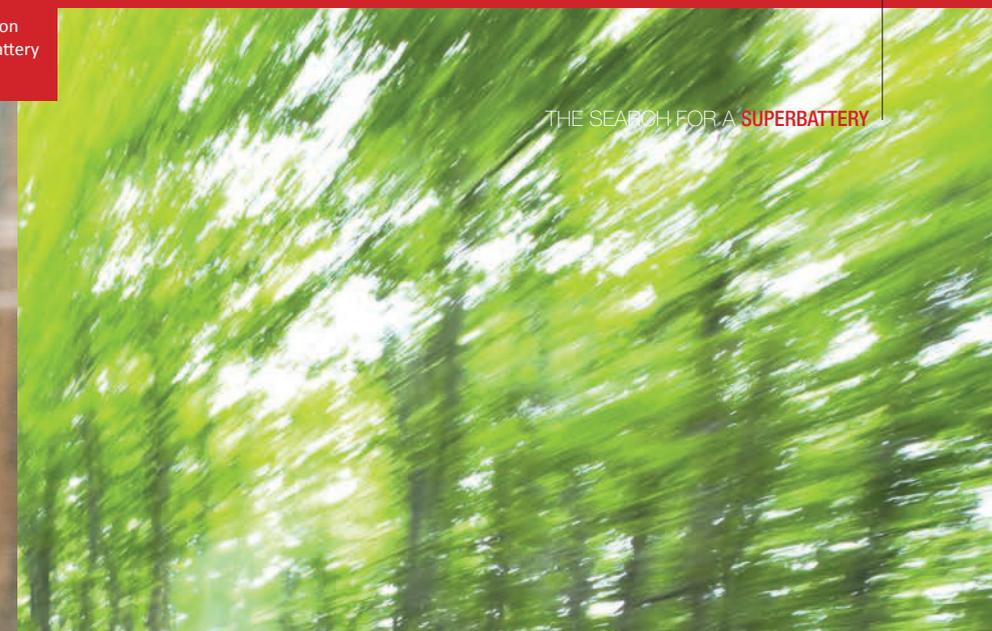
The United States could gain a lot by being the country where the next big battery is developed. If American companies and universities partner with national labs to grow and distribute the technology, the breakthrough could boost American manufacturing and create new jobs.

“Batteries are a large, heavy component of electric and hybrid cars, and so it’s best to manufacture them near the factory where the cars are assembled,” explained Jeff Chamberlain, who heads Argonne’s battery R&D. “This means cars assembled in U.S. factories will also need battery factories nearby—creating more American jobs.

“We’re developing technology that I’m highly confident will help make plug-in hybrid cars more economic,” he said. “The work at Argonne ends up in the hands of taxpayers who paid for research. This is a fulcrum, a key component to moving away from fossil fuels.”

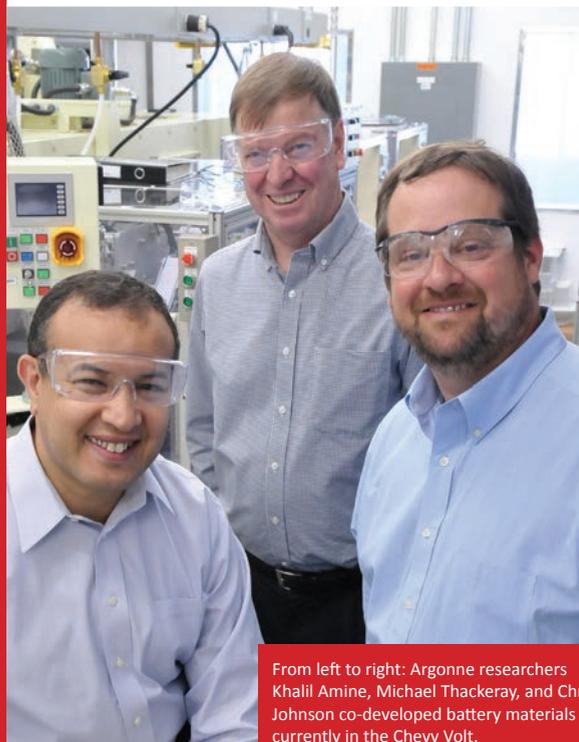


Argonne's Daniel Abraham holds a lithium-ion cell that's being tested to determine why battery performance deteriorates.



CATCHING THE WIND

Better batteries aren't just great for cell phones; they're also key to moving us to renewable energy sources. Since the sun doesn't always shine and the wind doesn't always blow when we need power, in order to depend on them we need to be able to stock up on electricity when we can. Right now, there's no good universal way to store large amounts of energy—lithium batteries just cost too much in large quantities—but dedicated R&D should change that. Some have even suggested recycling used lithium car batteries as electric grid storage.



From left to right: Argonne researchers Khalil Amine, Michael Thackeray, and Chris Johnson co-developed battery materials currently in the Chevy Volt.

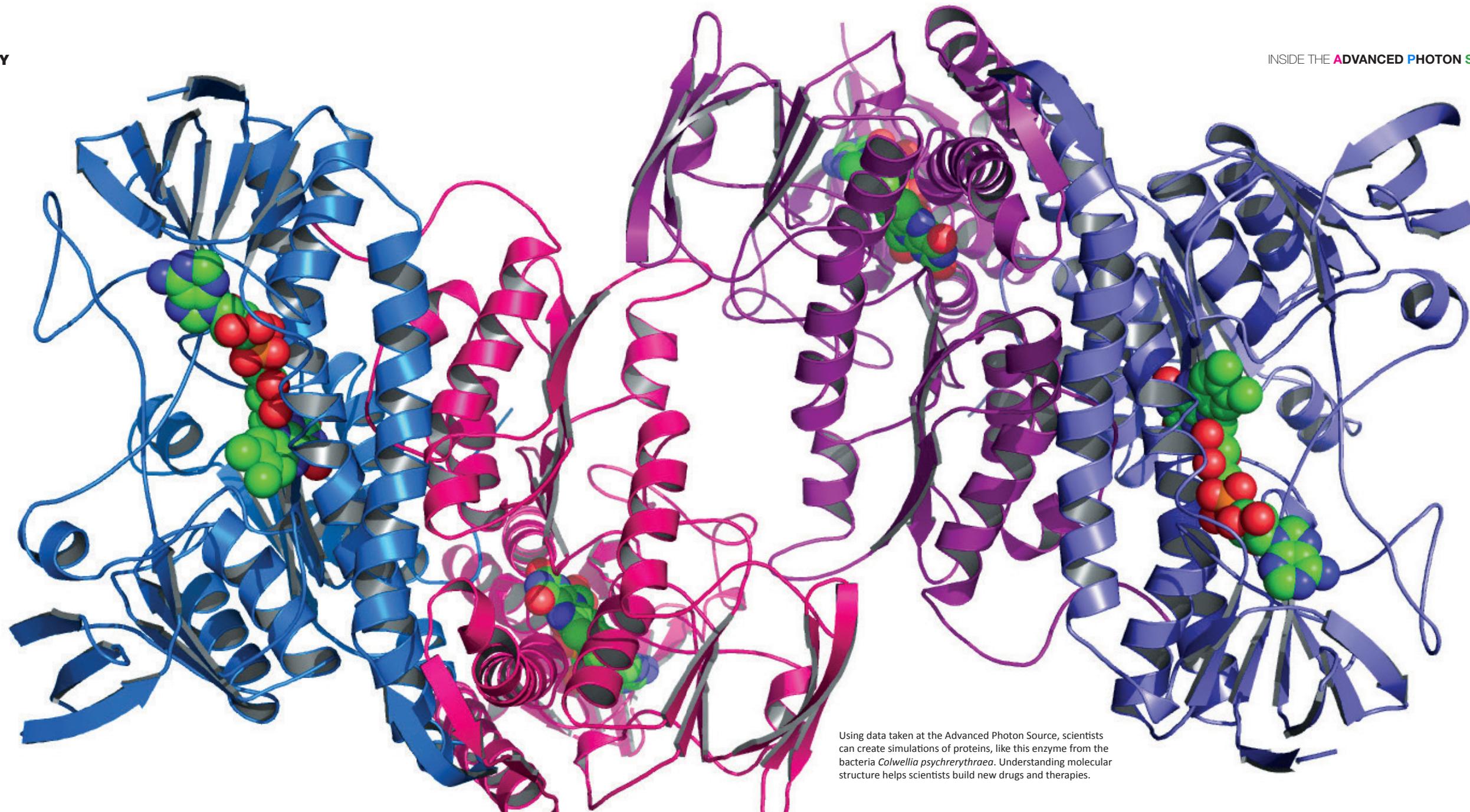
BANDING TOGETHER FOR BATTERIES

Michael Thackeray is the director of one of the Department of Energy's Energy Frontier Research Centers, called the Center for Electrochemical Energy Storage. Argonne is the lead, along with partners Northwestern University and the University of Illinois at Urbana-Champaign. The center is receiving \$19 million over five years to tackle problems with today's lithium-ion batteries, especially understanding and overcoming the limitations of electrochemical reactions at electrode interfaces, which play a critical role in controlling battery performance, life, and safety. Read more at Argonne's website: www.anl.gov/energy-storage-science



Argonne chemist Chris Johnson studies materials for batteries.





Using data taken at the Advanced Photon Source, scientists can create simulations of proteins, like this enzyme from the bacteria *Colwellia psychrerythraea*. Understanding molecular structure helps scientists build new drugs and therapies.

by Jared Sagoff

INSIDE THE **A**DVANCED

Access the atomic level at Argonne's giant synchrotron. **P**HOTON

SOURCE

To see inside Argonne's Advanced Photon Source, all it takes is a little bit of light.

The electrons traveling around the kilometer-long electron storage ring generate extremely powerful X-rays that penetrate to the heart of some of our country's most complicated scientific questions.

Virtually every day, around the clock, scientists around the ring are simultaneously working on experiments in many different fields: materials science, protein biology, environmental science, chemistry, and nanotechnology, to name just a few.

The **APS**
is supported by the
U.S. Department of Energy's
Office of Science.



This is possible at the Advanced Photon Source (APS) because it simultaneously generates X-rays at 34 different sectors, each containing one or more beamlines—which means that dozens of different experiments are going on at any given moment. Every year, thousands of users from industry, academia, and government laboratories come to Argonne to perform experiments at the facility.

The APS, one of the world's most powerful X-ray sources, produces pulses of light that are both extremely bright and penetrating. Together, these qualities let scientists look at all kinds of remarkable structures under different conditions, pressures, and temperatures.

BIGPharma, Tiny Protein

Several of the beamlines at the APS cater to users who come to Argonne from the pharmaceutical industry. Many new drugs that wind up on pharmacy shelves are inhibitors, which prevent the action of key cellular enzymes involved in certain diseases. The way that these enzymes work is by latching onto other molecules; if you can block the “active site” where that happens, the enzyme protein can't work.

To make a new drug, scientists build an inhibitor to precisely block that site—but they often have to be fashioned molecule-by-molecule, like making a key to fit into a lock. The first step is knowing what the lock looks like.

To get a picture of the protein's structure, researchers bring tiny samples of crystallized protein to the APS, where they are loaded onto small pins and exposed to the APS X-rays. The patterns recorded by the beamline's detector can

be interpreted to determine the positions of individual atoms within the sample. Research done at the APS has resulted in the development of drugs that treat HIV/AIDS (Kaletra®) and melanoma (Zelboraf®) and led to new insights into the structures of the viruses that cause HIV, influenza, swine flu, and even the common cold.

One of the sectors at the APS is owned and operated by Eli Lilly, the fifth biggest pharmaceutical company in the United States. Another, known as IMCA-CAT, is owned and operated by the Industrial Macromolecular Crystallography Association, a consortium including Merck, Pfizer, Bristol-Meyers Squibb, Novartis, and Abbott Laboratories.

REAL Materials, REAL Conditions

One of the major advantages of the X-rays produced by the APS is that they allow scientists to study materials *in situ*—that is, in conditions that replicate the natural environment. For example, researchers can examine how a catalyst will react at different temperatures or pH.

A little ways farther around the APS ring, Argonne chemist Peter Chupas and his colleagues look at the performance of battery components at the X-ray Science Division's Sector 11 beamlines.

“Years ago, we could only take one battery and cycle it very slowly, but now in the same amount of time we

can investigate ten batteries,” Chupas said. “By getting more information we can understand entire battery systems; we can get the real hard numbers on their performance so that we can go back to our models and improve our predictions about their behavior.”

The X-ray beams at Sector 11 are both strong enough to penetrate all the way into a battery and narrow enough so that researchers can pick out specific regions to investigate. These narrow beams allow scientists to take data from many different points on the sample, creating a richer picture of a material's structure and function.

Like all of the APS beamlines, Sector 11 is used year-round by academic and industrial groups who come to the facility to try to bridge the gap between the fundamental properties of materials and fully mature technologies. “What separates us from the pack is the fact that we're able to do these very precise and fundamental measurements on an applied system,” Chupas said. “We're always looking for new ways to combine the two.”

Argonne researchers are continually improving the instruments on the beamlines to provide users with the best technology available. “We're developing new tools constantly,” Chupas said.

HONEY, I Shrunk the Beam

The ability to condense beam sizes ever further has also yielded benefits at a life science beamline where researchers work on targeted drug design, especially for treating cancer.

The development of the hard X-ray minibeam quad collimator, which earned an R&D 100 award in 2010, has let scientists shrink the beam diameter—from 20 microns down, in some cases, to a single micron. That's thinner than a strand of spider silk.

The beamline is funded by the General Medicine and Cancer Institutes of the National Institutes of Health.

In one of the most challenging experiments at this beamline last year, researchers from Stanford University and other institutions wanted to study a type of protein called G-coupled protein receptors, a frequent drug target. Specifically, they wanted to study a protein that's part of an elusive but extremely important multiprotein complex.

The crystallized proteins are essentially invisible to the eye, which makes them difficult to position within the X-ray beam. The team had to create special computer software to scan the samples.

This beamline has also facilitated research on adenovirus, a virus of interest not only for its role in the common cold and other respiratory

diseases, but also for its potential for gene-delivery methods for treating serious diseases like cancer. More information on that study can be found on page 54.

LIGHTING up the future

Even though the APS already produces some of the brightest X-rays in the Western Hemisphere, Argonne engineers and physicists are already planning to make the facility even more powerful by dramatically improving the brightness, sensitivity, and resolution of the synchrotron.

A proposed upgrade to the APS, which received a preliminary go-ahead from Congress, has already entered the design phase. This year,

“Each pulse can be thought of as a single exposure, like a snapshot,” said Linda Young, director of the X-ray Sciences Division at Argonne. “With shorter pulses, you can freeze the motion of faster processes—such as molecules reconfiguring under the direction of laser light.”

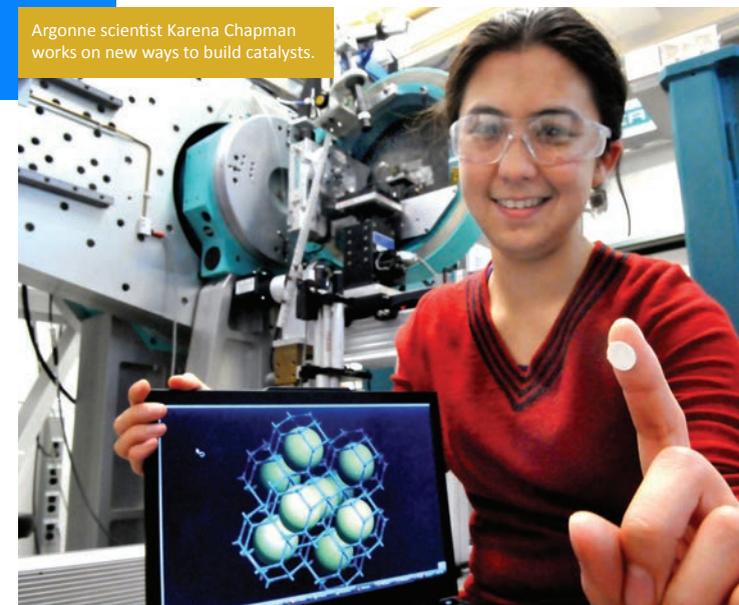
Right now, the APS generates X-ray pulses that are approximately 100 picoseconds long—that's just one-tenth of a nanosecond—but researchers at the facility are trying to reduce that by a factor of nearly one hundred.

“We're just in the first phases of what we hope will result in the creation of a machine capable of exploring a wider range of materials and phenomena than ever before,” said project director George Srajer.

In addition to the APS Upgrade, the APS will gain a brand new beamline—the only one of its kind—to explore shock physics: the branch of science that studies what happens to materials when they're exposed to large stresses in very short periods of time.

“The whole point of the upgrade is to provide more flexibility for our users so that they have access to state-of-the-art investigative tools, now and in the future,” Srajer said. ✨

APS.ANL.GOV



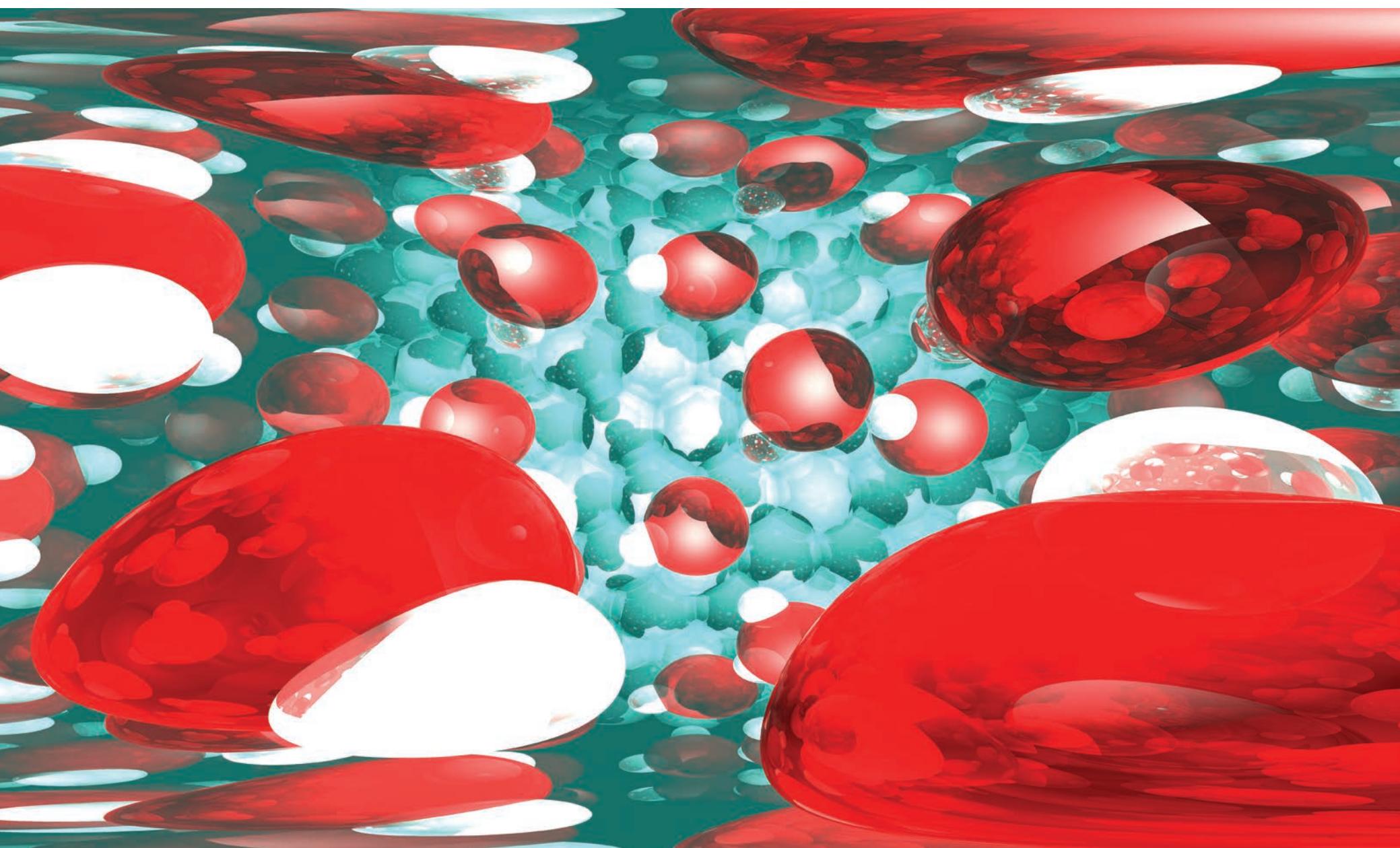
Argonne scientist Karena Chapman works on new ways to build catalysts.



7 THINGS

you may NOT KNOW about CATALYSIS

by Louise Lerner



1 Catalysts are all around us.

Catalysts are one of those things that few people think much about, beyond perhaps high school chemistry, but they make the world tick. Almost everything in your daily life depends on catalysts: cars, Post-It notes, laundry detergent, beer. All the parts of your sandwich—bread, cheddar cheese, roast turkey. Catalysts break down paper pulp to produce the smooth paper in this magazine. They clean your contact lenses every night. They turn milk into yogurt and petroleum into plastic milk jugs, CDs, and bicycle helmets.

2 Catalysts are like cheat codes for chemistry.

Catalysts speed up a chemical reaction by lowering the amount of energy you need to get one going. Catalysis is the backbone of many industrial processes, which use chemical reactions to turn raw materials into useful products. Catalysts are integral in making plastics and many other manufactured items.

Even the human body runs on catalysts. Many proteins in your body are actually catalysts called enzymes, which do everything from creating signals that move your limbs to helping digest your food. They are truly a fundamental part of life.

3 Small things can have big results.

In most cases, you need just a tiny amount of a catalyst to make a difference. Even the size of the catalyst particle can change the way a reaction runs. Last year, an Argonne team including materials scientist Larry Curtiss found that one silver catalyst is better at its task when it's in nanoparticles just a few atoms wide. (The catalyst turns propylene into propylene oxides, which is the first step in making antifreeze and other products.)

4 It can make things greener.

Industrial manufacturing processes for plastic and other essential items often produce nasty by-products that can pose hazards to human health and the environment. Better catalysts can help solve that problem. For example, the same silver catalyst actually produces fewer toxic by-products—making the whole reaction more environmentally friendly.

At its heart, a catalyst is a way to save energy. And applying catalysts on a grand scale could save the world a lot of energy; 3% of all of the energy

used in the U.S. every year goes into converting ethane and propane into alkenes, which are used to make plastics, among other things. That's the equivalent of more than 500 million barrels of gasoline.

Catalysts are also the key to unlocking biofuels. All biomass—corn, switchgrass, trees—contains a tough compound called cellulose, which has to be broken down to make fuel. Finding the perfect catalyst to disintegrate cellulose would make biofuels cheaper and more viable as a renewable energy source.

5 Often, we have no idea why they work.

The precise reasons why catalysts work are often still a mystery to scientists. Curtiss works in computational catalysis: using computers to tackle the complicated interplay of physics, chemistry, and math that explains how a catalyst operates. Once they've figured out the process, scientists can try to build a catalyst that works even better by simulating how different materials might work instead. Potential configurations for new catalysts can run to thousands of combinations, which is why supercomputers are best at dealing with them.

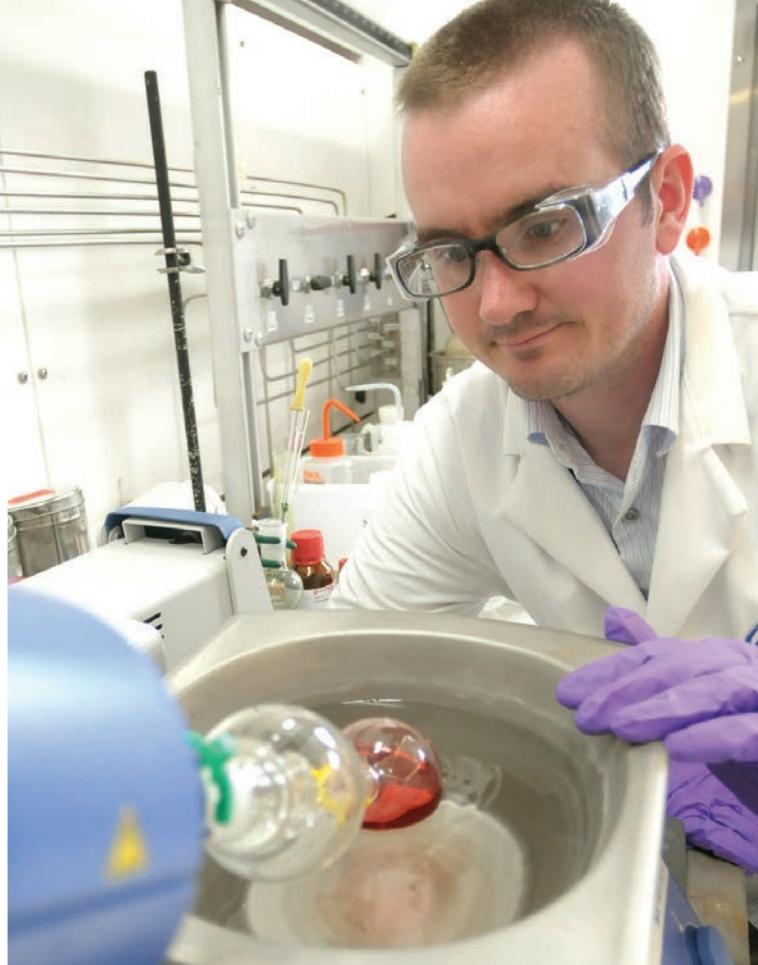
When Edison was building the lightbulb, he tested literally hundreds of different filaments (likely testing the patience of his lab assistants as well) before discovering the carbonized filament. By taking advantage of supercomputers and modern technology, scientists can speed up the years of testing and expense to get to breakthroughs.

Curtiss runs simulations on Argonne's Blue Gene/P supercomputer to design possible new catalysts. "As supercomputers have gotten faster, we've been able to do things we'd never have been able to do 10 years ago," he said.

>>> *continued*



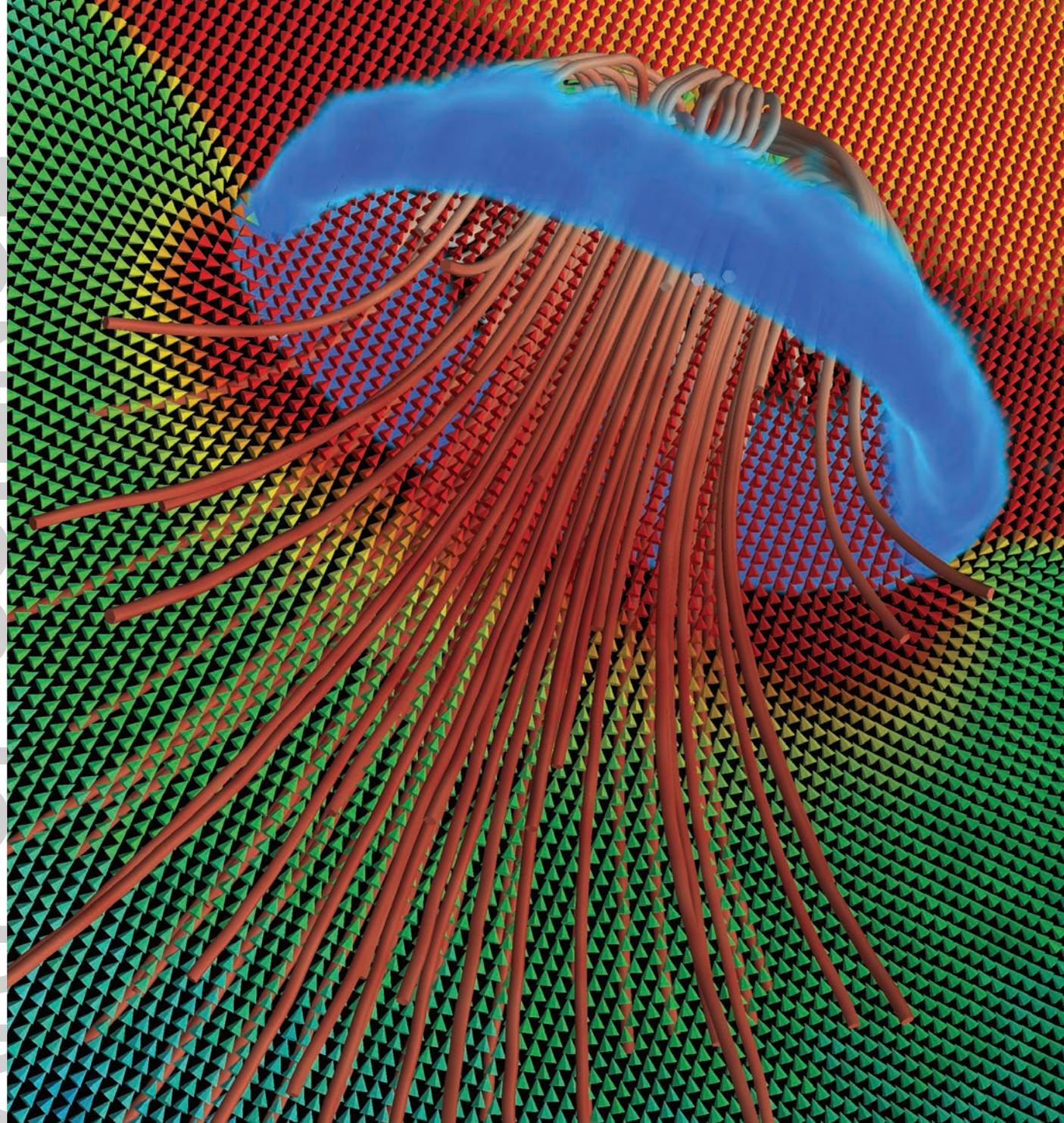
Argonne postdoctoral students Worajit Setthapun (left) and Ryan Nelson synthesize and test new catalysts.



6 They could be essential for the next big revolution in batteries. Newly efficient lithium-ion batteries helped turn clunky car phones into the slim, elegant cell phones and laptops available today. But scientists are already searching for the next revolution in batteries—one that could someday make a battery light and powerful enough to take a car 300 miles at a go. A promising idea is lithium-oxygen batteries, which use oxygen from the air as a primary component. But this new battery will require totally revamping the internal chemistry, and it will need a powerful new catalyst to make it work. A lithium-oxygen battery works by combining lithium and oxygen atoms and then breaking them apart, over and over. That is a situation tailor-made for a catalyst, and a good one would make the reaction faster and the battery more efficient.

7 Big scientific facilities can help us find the next one. Understanding the chemistry behind reactions is the first step; then scientists can use modeling to design potential new catalysts and have them tested in the lab. But that first step is difficult unless you can get down to the atomic level to see what is happening during a reaction. This is where big scientific facilities like Argonne's Advanced Photon Source shine. At the APS, scientists can use extremely bright X-rays to track the reactions in real time. At the laboratory's Electron Microscopy Center, researchers take photos of the atoms while they react. Curtiss and the team have used both of these in their search for better catalysts. ❄

ART OF SCIENCE



Scientists believe that phenomena called **"nanobubbles"** play key roles in several important chemical reactions. Nanobubbles are tiny—often smaller than the width of a single cell wall in your body—and when they collapse, they generate small shock waves. The combined force of many of these collapses may contribute to damage in ship propellers, pipes, and the blades of pumps. The goal of this nanobubble collapse simulation, which ran on Argonne's supercomputer, is to improve both the safety and longevity of materials in nuclear reactors.

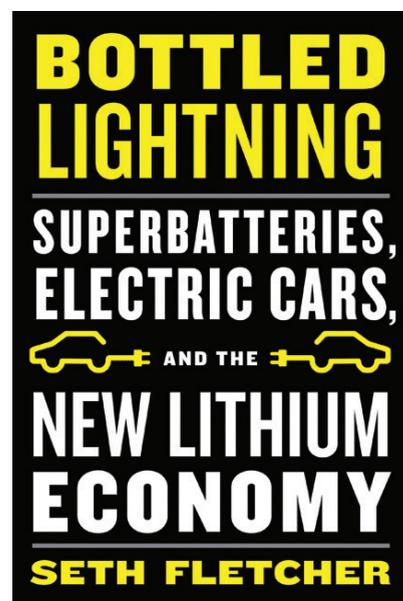
Data by Priya Vashishta, Rajiv K. Kalia, Aiichiro Nakano, Ken-ichi Nomura, Adarsh Shekhar (University of Southern California); image by Joseph Insley (Argonne National Laboratory).

ASSAULT ON BATTERY

The promising, frustrating, indispensable race by government and industry to revolutionize the storage of electricity.

By Eric D. Isaacs | Director, Argonne National Laboratory

BOTTLED LIGHTNING: Superbatteries, Electric Cars, and the New Lithium Economy by Seth Fletcher Hill & Wang, 272 pp.



Just five years ago, the documentary film *Who Killed the Electric Car?* claimed to prove conclusively that American electric vehicle technology had been effectively buried by an unholy cartel of car makers, government bureaucrats, oil companies, and SUV-loving consumers. The documentary's hard-hitting reporting and acerbic style persuaded thousands of moviegoers

that American industry would never allow an electric car to challenge the supremacy of the internal combustion engine.

That wasn't just the opinion of a few cranky independent filmmakers: the electric car has been a running joke on *The Simpsons* for years. (On a family trip to a theme park, Homer and Bart visit the Electric Car of the Future attraction—sponsored by the Gasoline Producers of America. On the ride, their sad, pastel-pink vehicle whines, "Hello, I'm an electric car. I can't go very fast or very far.")

But now, GM's Chevy Volt is being rolled out in cities across the country—and has been honored by *Motor Trend* as the 2011 Car of the Year: "A Car of the Future You Can Drive Today." Other car makers are racing to get their electric cars on American roadways: the Nissan Leaf is already in American markets; Toyota has unveiled a plug-in Prius; Mitsubishi is bringing its i-MiEV electric vehicle to U.S. dealers this year; and an electric Ford Focus is now available as well. These battery-powered vehicles are generating so much buzz that the producers of the 2006 documentary have been forced to make a sequel—*The Revenge of the Electric Car*.

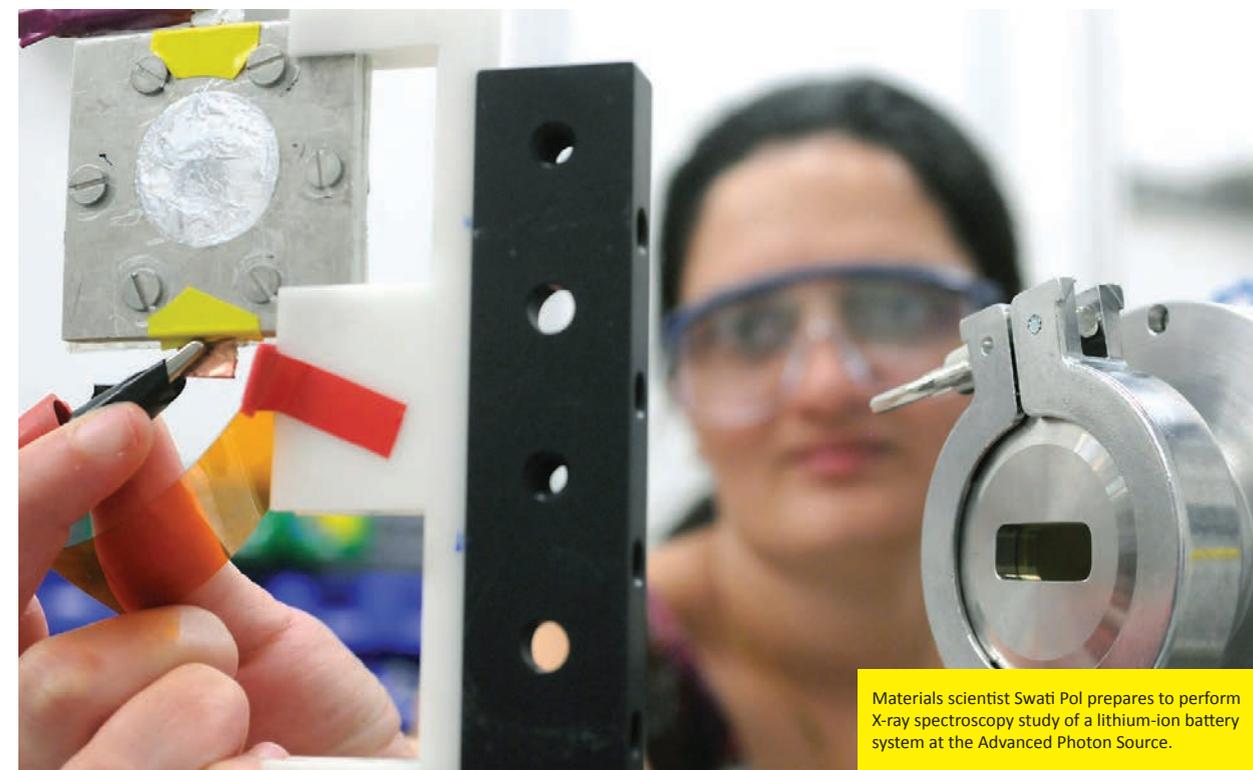
How did electric cars come so far, so fast? And, more important, both for consumers and for the

future of our country, where will they go from here? These are the questions posed—and at least partially answered—in *Bottled Lightning: Superbatteries, Electric Cars, and the New Lithium Economy*, by Seth Fletcher, a senior editor at *Popular Science* magazine. In this well-written, accessible history of lithium batteries and their role in the development of practical electric cars, Fletcher makes a strong case that new energy storage technologies are the key to a green industrial revolution.

"Electricity," Fletcher explains, is "the cleanest and most flexible" alternative to gasoline. "It's piped into every home in the country. Mile by mile, it's cheaper compared with gasoline...It can come from almost any source—natural gas, coal, nuclear, hydroelectric, solar, wind."

There's just one problem: it's hard to store. So if we want electric cars that aren't powered by extension cords, we need to build better batteries.

Historically, cars have been equipped with lead-acid batteries—heavy, environmentally unfriendly, and limited in storage capacity. Seeking a better alternative, scientists started "scouring the periodic table," in Fletcher's words, experimenting with various exotic chemical compounds before turning their sights on lithium, the lightest metal



Materials scientist Swati Pol prepares to perform X-ray spectroscopy study of a lithium-ion battery system at the Advanced Photon Source.

in the universe. Lithium's "eagerness" to shed electrons, along with its light weight and energy density, have made it the basis for the small, powerful batteries that now power billions of cell phones, laptops, and iPods; lithium-based batteries have the theoretical potential to challenge, pound for pound, the energy and power stored in gasoline.

FOR MORE ON THE SEARCH FOR THE SUPERBATTERY, TURN TO PAGE 32.

But there's a major gap between that theoretical energy storage and even the best lithium-based batteries available today. Thus far, no one has invented advanced battery technologies that can rival the price, reliability, and energy storage capacity of a tank of gas. And building a better battery is only

a first step toward reinventing our entire energy infrastructure.

But while the challenge is great, the potential rewards are enormous. If all of our cars and light trucks ran on electricity, we could cut American oil consumption by more than a third—roughly 7.2 million barrels of oil a day. Just as important, we could create tens of thousands of new green tech jobs in the long run—jobs that would stay right here at home. The implications for our global environment and our national energy security are enormous. But, as Fletcher warns, we can't hope to reach those goals without strong, consistent investment in developing new energy technologies, including next-generation battery systems.

As the director of a national laboratory, I have a deep-seated personal and professional interest in the future of energy research. And—like Fletcher—I see increasing reason for optimism about the potential of

lithium-based batteries to transform our energy economy.

The economic potential of these "superbatteries" is immense: the research firm IHS Global Insight predicts that **advances in battery technology will allow hybrids and electric cars to grab up to 15% of the world's new car sales by 2020.** At today's production rates, that's about 7.5 million cars a year.

But as Fletcher makes clear, the story of electric cars, and the battery technologies that power them, has been, in his words, "a parade of extraordinary failures stretching back to the late nineteenth century." The first electric cars date to the time of Thomas Edison, when the quiet and sedate electrics were considered "ladies' cars." > > > *continued*



Argonne scientist Ira Bloom prepares to open a lithium-ion cell at the lab's facility to test battery performance.

(In fact, Henry Ford's wife, Clara, bought an electric brougham in 1914 because she considered her husband's Model T too noisy.) Interest in electric vehicles has cyclically flared up every few decades ever since, usually in response to a spike in oil prices. But when gasoline costs have fallen, so has American consumers' willingness to trade in their gas guzzlers for electric cars—at least, for the electric cars that have been available until now.

Fletcher does a great job of walking readers through the history of battery technology, and he writes about the complexities of science and engineering with clarity and flair. He sums up the fundamental challenge of energy storage technology in one pithy sentence: "You can't just shove loose electrons in a can."

He's equally at ease describing the effects of America's roller-coaster energy policy, which has led to repeated cycles of brisk acceleration and sudden unexpected stops in our battery research programs. When it comes to energy technology research, as former Energy Secretary James Schlesinger once said,

"We have only two modes—complacency and panic."

Over the decades, complacency has tended to muffle interest in energy innovations. In 1979, in inflation-adjusted dollars, the federal budget invested about \$7.8 billion in energy-related research. In fiscal year 2010, that investment had fallen to \$5.1 billion. That figure represents a substantial increase over the budgets of the previous decade,

but it's still woefully short of the \$16 billion annual national investment recommended by the President's Council of Advisors on Science and Technology.

Today we find ourselves in an international race to create—and manufacture—viable lithium-based car batteries. For now, at least, it appears that the United States is a serious contender. A recent report by a veteran consultant to the battery industry compared all costs of manufacturing batteries in China and the United States, and found that U.S. manufacturing can be cost-competitive. Advanced battery manufacturing is highly automated, which reduces the Chinese advantage of low-cost, low-skilled labor; the salaries of highly educated, skilled workers to run the factories are roughly equivalent. Chinese

utility costs are twice as high as ours here in the United States. Add in the cost of shipping big, heavy car batteries around the world, and you've got a real market opportunity for U.S. battery makers.

As Fletcher's history teaches us, however, an opportunity is not a sure thing. The playing field could be tilted dramatically by foreign government investment—like the \$30 billion in low-cost loans the China Development Bank provided to Chinese solar manufacturers last year. If China or another foreign government makes that type of massive investment in lithium battery manufacturing, yet another great U.S. research breakthrough could wind up being commercialized and developed into a thriving new industry far from home.

Those risks are real. But the grim prospect of losing yet another new high-tech industry to foreign

competitors makes those risks worth taking. With affordable capital to cover the up-front costs of building advanced battery manufacturing plants factories here, I believe we have a real chance to be competitive in a large and growing world market—once we have the lithium battery technology to challenge the internal combustion engine. And that, of course, is the challenge at the heart of *Bottled Lightning*.

We still have a long way to go to create a battery system that can rival the energy stored in a tank of gas. We have to solve some knotty scientific puzzles, using technology we haven't invented yet. For example, we know that a battery using air as a cathode could offer energy density up to ten times higher than today's lithium-ion batteries. But first, we have to discover a way to make a battery that "breathes in" oxygen from the air to discharge

electricity, then "breathes out" again to recharge. Then we have to convert those discoveries into battery systems that can be affordably mass-produced and put these technologies into cars that consumers want to buy, and we have to do it all before our international competitors catch up. But, as Fletcher comments, "[t]here are a couple of ways to react to this sort of discouraging calculus. One is defeatism. The other is research."

Fletcher understands that, ultimately, this is a battle of economics, not technology: "Dollars per kilowatt-hour stored is all that matters." Our long-term goal is to create car battery systems that are smaller, sturdier, and about ten times more powerful than the ones we have today. But as one analyst told Fletcher, if the price of the current generation of car batteries comes down far enough—or if the price of gasoline goes high enough—"It's game over for gasoline."

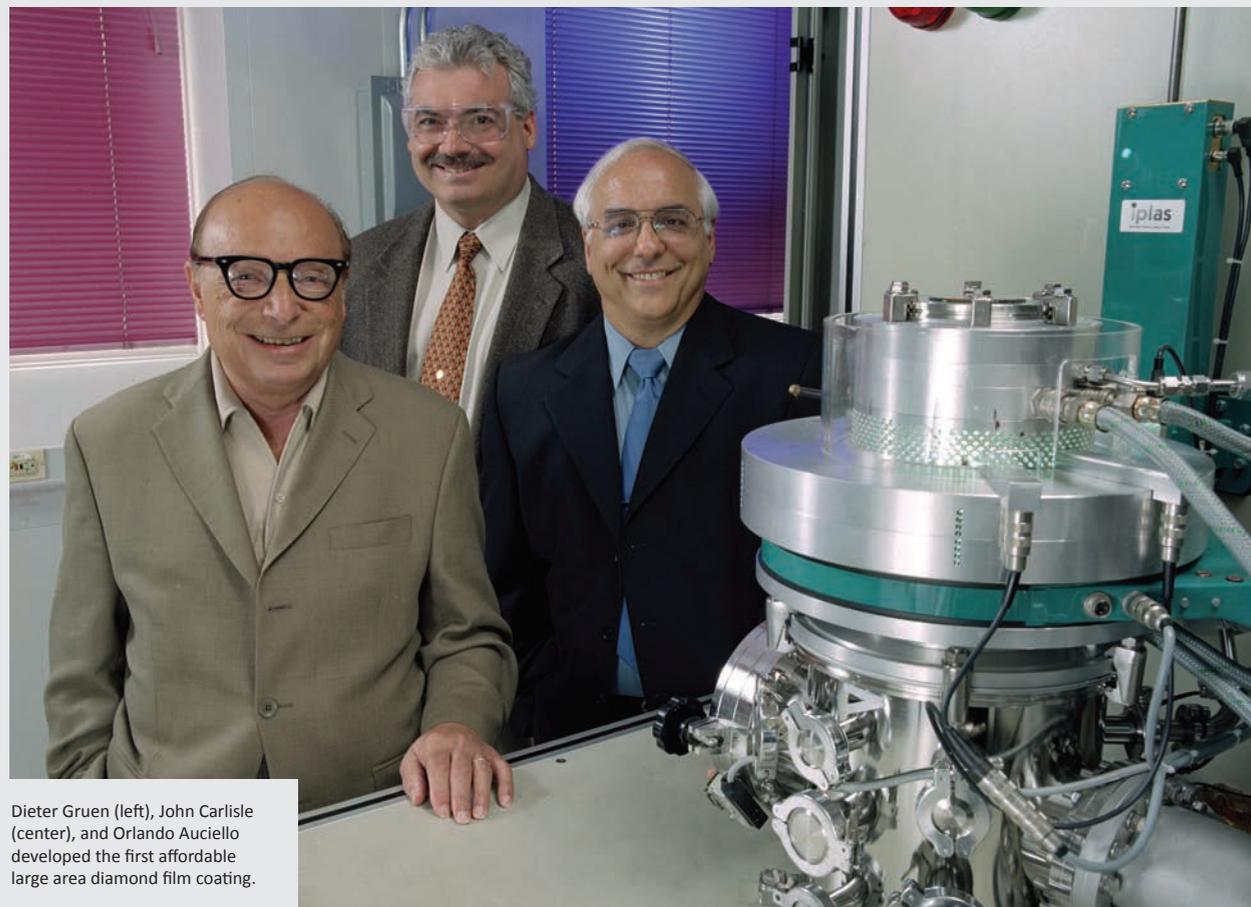
Looking ahead, I hope Seth Fletcher and his colleagues will continue to beat the drum for battery R&D, and will keep on working to inform the American public about the potential for lithium technologies to create new jobs, recharge our nation's manufacturing base, and help us build a new, secure, green energy economy. As Fletcher concludes, "If the budding American energy-storage industry fails ... it would be a tremendous lost opportunity, a failure to participate in what promises to be one of the greatest industries of the coming century."

A version of this book review appeared in The Washington Monthly.



Argonne researcher Ilias Belharouak monitors the fabrication of electrode materials for use in plug-in hybrids' energy storage systems.

Originally discovered when an Argonne scientist introduced buckyballs into a microwave plasma machine, tiny diamond sheets are now commercially available.



Dieter Gruen (left), John Carlisle (center), and Orlando Auciello developed the first affordable large area diamond film coating.

ULTRANANOCRYSTALLINE DIAMOND: A THIN SHEET OF DIAMOND HAS WORLDS OF USES

Even as royalty set diamonds into crowns and rings, engineers lusted after the gems for different reasons: diamonds are harder than any other natural material and are excellent electrical insulators and heat conductors. Today they are widely used in industry and factories. But the diamond supply is limited, and while you can make artificial diamonds in gem form, they have been hard to synthesize in thin films.

A technique invented at Argonne creates thin films of diamond with grains so small they're called ultrananocrystalline diamond (UNCD®) films. The films can be applied to an astounding array of surfaces and uses, ranging from better seals on pumps to heart pump walls so smooth that dangerous blood clots don't form. The grains of diamond in the film are just five nanometers across—about a billion of them would fit inside one red blood cell.

UNCD captures most of the natural properties of diamond. The films are harder than any other diamond film demonstrated today; they are extremely smooth and chemically inert—so they don't interact with other substances—and they are good electrical conductors when doped with nitrogen or boron. Each film can be precisely tailored.

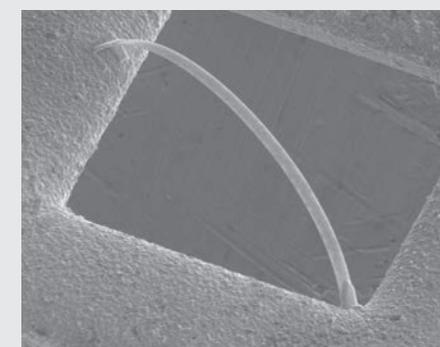
Advanced Diamond Technologies Inc., in Romeoville, Illinois, formed as a start-up company spun out of Argonne in order to manufacture

UNCD products. For example, if you coat mechanical pump seals with UNCD, the film is so smooth that it reduces friction and saves up to 20% of the energy used to run the pump. The coating has also been successfully used on atomic force microscope tips and bearings in industrial mixers.

The U.S. Department of Defense is working with the company to use the films in sensors that would take quick readings to detect chemical and biological threats in water. The films can be treated to bond with biomolecules like *E. coli*, *Salmonella*, *Listeria*, and other pathogens in water to detect their presence. The goal is to miniaturize the detectors so that anyone, including soldiers, police, or public health officers, could carry them.

Finally, because diamond is chemically inert, it doesn't react with biological human tissue or body fluids—and the body doesn't reject the diamond as a foreign material. For this reason, UNCD can be used in implants, including artificial retinas and heart pumps to treat heart failure.

www.anl.gov/technology



This ultrananocrystalline diamond nanobelt is just 100 nanometers thick—half the size of a single bacterium.



When coated with ultrananocrystalline diamond, these pump seals use less energy during pumping.

Interested in commercializing these or dozens of other available Argonne technologies? Contact partners@anl.gov or visit www.anl.gov/technology.

AVAILABLE FOR LICENSING

Many more Argonne innovations are available for licensing. Here's just a few:

CLEANER DIESEL EMISSIONS

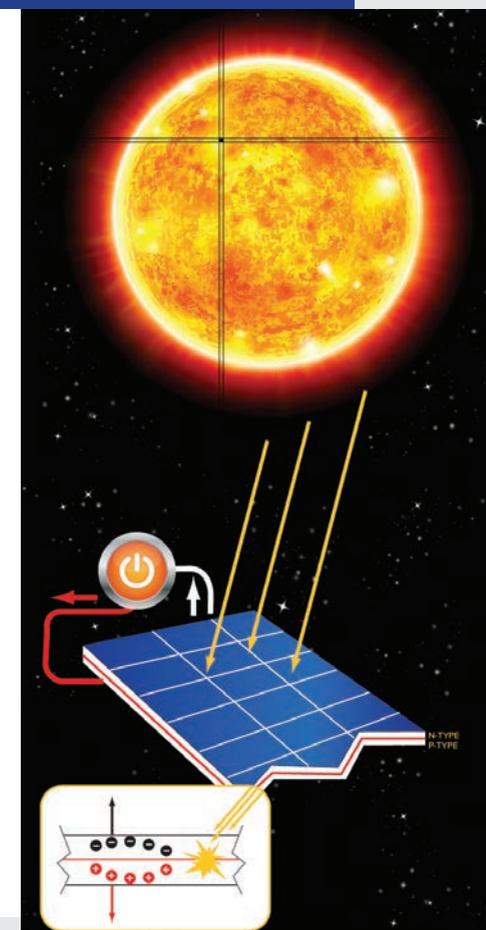
The diesel DeNOx catalyst removes 80–85% of nitrogen oxide emissions from diesel fuel combustion. Inexpensive and easy to install, the catalyst can also be retrofitted to older engines.

RENEWABLE METHANE

This low-cost process accelerates methane production rates at least fivefold at wastewater treatment plants, farms, and landfills.

CHEAPER SOLAR CELLS

A technique called atomic layer deposition shows promise for a dramatic performance improvement in photovoltaic solar cells.



Funding for original research was provided by the Department of Energy Office of Science, Office of Basic Energy Sciences; later funding came from the Defense Advanced Research Project Agency, Office of Naval Research, and National Science Foundation.

THE SECRET LIVES OF NUCLEAR SCIENTISTS

Reprinted with permission from "Clever Apes," a radio series hosted by National Public Radio's Gabriel Spitzer on WBEZ – Chicago.

In pop culture, we tend to pigeonhole scientists into a few stereotypes: out-of-touch nerds (Jerry Lewis' Nutty Professor), bumbling head-in-the-clouds types (Doc Brown) or obsessed madmen (Dr. Frankenstein). Which is what makes it so much fun to pull back the curtain on the secret identities of a couple of local players in nuclear science.



Marius Stan

SPITZER: On this edition of *Clever Apes*, we reveal the secret lives of nuclear scientists. I find that in almost every case there's something more than meets the eye, and that's certainly the case for the gentleman I'm here with now. Could you introduce yourself, Marius?

STAN: Sure. My name is **Marius Stan**. I'm a physicist and a chemist by training, but I've been working on computational materials science for quite a while.

SPITZER: And these would be materials that might form components of, say, a nuclear reactor?

STAN: That is true. I have a keen interest in imperfection, in people and in materials. I think imperfections give character to a material.

SPITZER: All right, that's sort of your Clark Kent persona. But you have a whole other life.

STAN: I'm also an actor, most recently in the AMC series *Breaking Bad*.

SPITZER: So your character's name is Bogdan and he's the guy that owns the car wash. That's a fairly major role here in this fourth season. Are you an actor?—I mean, a trained actor—have you always been an actor?

STAN: No, it kind of happened by accident. This is a parlor life.

SPITZER: How on earth did it happen?



Chemistry teacher turned meth manufacturer Walter White (Bryan Cranston), left, and Bogdan (Marius Stan) in HBO's *Breaking Bad*.

STAN: I was accompanying my daughter to an audition. It happened that the casting director for that movie needed somebody to say one line in the pilot episode of *Breaking Bad*, and they thought I had the looks and the voice for one line. Then they decided to make it a recurring character.

SPITZER: So did they ever tell you what it was about you that made you such an appealing actor for them?

STAN: There are various opinions about that. Some people say it's because I have big eyebrows and that makes me stand out in the crowd.

SPITZER: They are magnificent.

STAN: Thank you.

SPITZER: The program is about a scientist, a trained chemist, Walter White, who has this double life; of course in his case his double life is cooking meth on the side. You are a scientist with a bit of a double life yourself. Do you feel like there are parallels there?

STAN: Yes, there are. I sympathize with the main character in many respects. I think it's quite interesting and poses a number of questions of artistic nature—but also social. What do people have to do to maintain a family; what do they do when they get sick, or if they're desperate. Will I ever break bad, I ask myself. So, who knows?

SPITZER: Who knew Argonne National Lab was such a hive of shadowy double lives? Just a few buildings down from Marius Stan's office, we're about to uncover another secret identity. From 1964-2007, scientists here at the Alpha Gamma Hot Cell experimented on irradiated nuclear fuel. Through the windows you can see buttons and dials, stacks of cans, and big robotic arms cocked at the ready.



Dan Pancake is in charge of packaging up all of the uranium and plutonium inside and getting it out of here safely. Over the years, he's dealt with all kinds of stuff, from twenty thousand curies of cobalt-60 to biological samples from factory workers who painted glow-in-the-dark watch dials. Dan Pancake has been a waste guy—that's his term—for close to 10 years. But that's just a fraction of his eccentric resume. From four o'clock or so he ditches the radiation dosimeter and puts on his white chef's jacket.

PANCAKE: You'll be coming to our restaurant, *Autre Monde*, which means literally "another world" in French. It's past ironic, all the way back around to being exactly representative of what it is in my life.

SPITZER: Food critics recommend *Autre Monde's* grilled octopus with capers and vinaigrette, or the guinea-hen sausage with oil-cured olives. This high-end Mediterranean restaurant is just five months old, founded by Pancake, his wife Beth Partridge, and two other partners.

PANCAKE: Here we do things that are very simple and very elegant. But it's really very difficult, because the fewer ingredients you have on a plate, the more accurately you have to cook and season those few ingredients.

SPITZER: Not just anyone can oversee the handling of plutonium pallets in the afternoon and be supervising a pappardelle dish by evening.

ARANZA: Dan is an anomaly.

SPITZER: John Aranza is one of Pancake's partners and a friend dating back to their days at *Café Spiaggia*.

ARANZA: You know, he's kind of like Batman, he's got his day job and his night job. He's a little bit superstar, he's a little bit scientist.

SPITZER: Pancake works grueling hours...much like Batman. By eight or so, he's ready for a glass of bubbly wine from the bar.

PANCAKE: If you had to give me a job title, it wouldn't be 'senior nuclear technical specialist' and it wouldn't be 'chef'. It would be operations manager for both jobs.

SPITZER: In each case, Pancake is managing teams, designing systems, and solving problems. Like when he and a co-worker needed to sift some fine grains of nuclear fuel, but didn't have the right tools.



Dan Pancake

PANCAKE: So we're sitting there, and immediately my mind goes to kitchen equipment. In the office, because we have office parties, right—potlucks and stuff—we still have a couple of half sheet pans, a couple of half pans, a couple glazing racks, and a bus tub.

SPITZER: They designed an apparatus right there, took the cookware back to the shop, and broke out the welding torch.

PANCAKE: I'm not kidding, I have pictures on my phone of hot cell operators remotely using equipment that you just saw in the kitchen to separate irradiated fuel from the rest of the material in the hot cell. It worked 100%, and it cost the United States government nothing.

SPITZER: Equally at home in the hot cell or the hot grill, Pancake says he may not have planned this double life, but in ways that surprise even him, the two worlds seem to keep coming back together. ☼

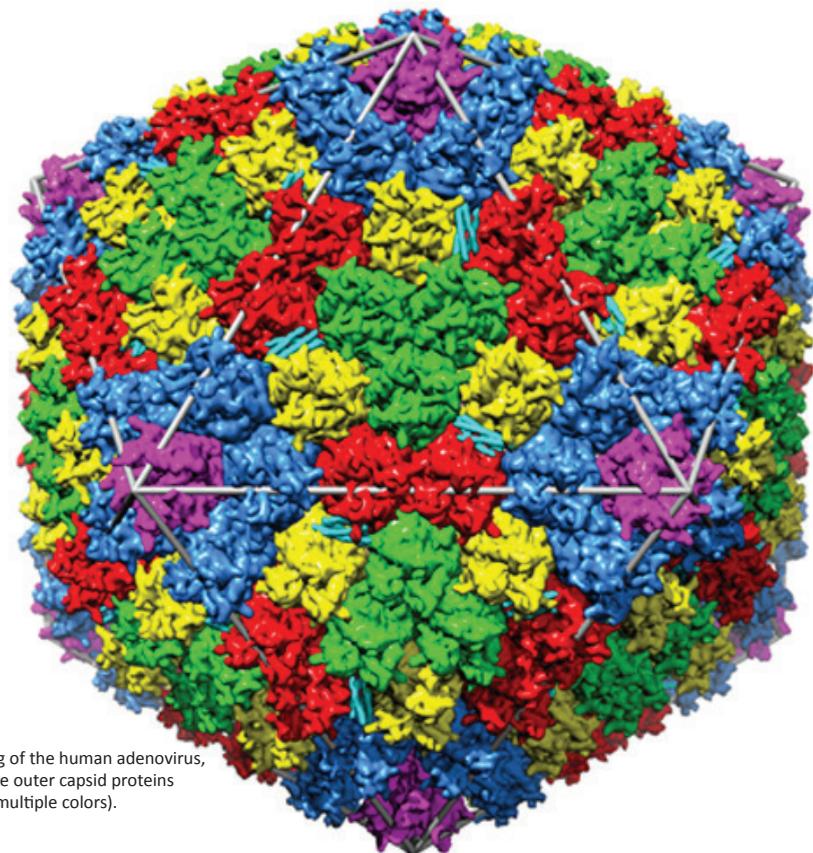
This is a transcription, slightly edited for length, from an episode of the WBEZ radio science series "Clever Apes". Find out more at www.wbez.org/cleverapes.

Marius Stan is a chemist, physicist, and computational materials scientist at Argonne National Laboratory, doing theoretical work and computer modeling on materials for nuclear reactors. He also has a recurring role on *Breaking Bad*.

Dan Pancake runs nuclear cleanup projects at Argonne, spearheading the technically complex work of removing radioactive uranium and plutonium from the lab. He's also a chef and restaurateur, owner of a new (and well-reviewed) fine-dining Mediterranean restaurant in Berwyn near Chicago.

chasing a COMMON COLD VIRUS

Every issue, we take a look at Argonne research on a different human disease or condition.



A rendering of the human adenovirus, showing the outer capsid proteins (shown in multiple colors).

By Susheela Bhat

As we prepare for the cold and flu season, a team of researchers using Argonne’s Advanced Photon Source continues to complete a detailed map of the human adenovirus—one of several viruses responsible for the common cold.

Although human adenovirus is usually not deadly, it is a seasonal nuisance to some and can cause deadly infections in others.

In the early 1990s, Glen Nemerow, professor and principal investigator at the Immunology and Microbial Science division of The Scripps Institute, switched from his previous research on Epstein-Barr to human adenovirus. “It is easy to grow and manipulate, which made (and makes) it an excellent model for studying host-cell interactions,” said Nemerow.

Although the virus had been studied since the early 1950s, most research tended to focus on subunits

of the virus, such as major proteins, because the intact virus is dauntingly large. Nemerow decided instead to examine the entire molecular structure of human adenovirus. He wanted to see how proteins self-assemble to form the complete virus. A major goal of the research is to try to improve how the virus could be used for gene delivery—and potentially, cancer therapy. Nemerow teamed up with Vijay Reddy, an associate professor at Scripps, to investigate the 3-D shape of human adenovirus using a technique called X-ray crystallography.

First the researchers needed to grow a crystal of the virus. This presented several challenges. For one, a complete human adenovirus sports fiber “spikes” that help it attach to a host cell but also prevented researchers from successfully growing a crystal. One of the first steps the scientists took

was to engineer a human adenovirus molecule without the fiber spikes. Altogether, getting usable crystals took five years.

When they were ready to test the virus crystal, Nemerow and Reddy partnered with Argonne biophysicist Robert Fischetti and started their work at the Advanced Photon Source’s General Medicine and Cancer Institute Structural Biology Facility GM/CA beamline.

Unlike other beamlines they’d tested, the GM/CA beamlines produce intense X-ray beams that allowed the researchers to collect high-quality data from the virus crystals. This gave researchers a detailed 3-D image of the structure—the largest structure of any biomolecule determined by X-ray crystallography to date.

“Without the beamline, we would have been stymied on this project,” said Nemerow. The APS beamline, they hoped, would reveal where electrons were clustered in the human adenovirus molecule and how they were connected.

Over the course of the project, Fischetti and colleagues modified the beamline to improve the uniformity of the beam. They installed smoother mirrors, reduced the amount of radiation damage to the crystals, and provided the team more flexibility to focus the beam. This helped Nemerow and Reddy hone the first electron density map of the human adenovirus’ structure, which they published in the journal *Science*.

Nemerow and Reddy compared their map to what was already known about the human adenovirus from previous research. “We weren’t able to assign an identity for all 12 of the proteins in human adenovirus to the electron density we mapped out,” Nemerow said. “There were also four major ‘cement’ proteins we could not identify or assign—either because they haven’t been seen yet, were too disordered, or because we didn’t have enough data at the time.”

Cement proteins, as their name suggests, bind major proteins to the virus shell, or capsid.

Nemerow and Reddy found major capsid proteins tended to be easier

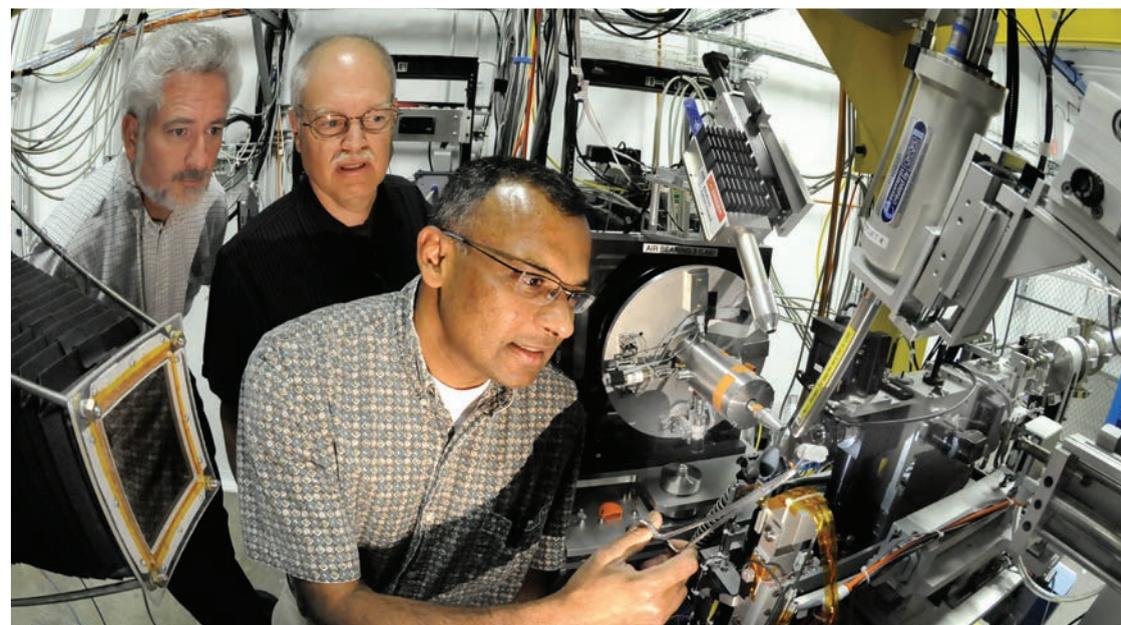
to see in an electron density map because of their symmetry and general stability, but cement proteins proved the sticking point. “We don’t know the structures of cement proteins at high resolution yet, because they are difficult to purify by themselves—which makes them even harder to crystallize,” Reddy explained. “The cement proteins bind to major capsid proteins, like cement to bricks, and mediate interactions between them.”

Because cement proteins are flexible and dynamic, they can degrade easily from radiation damage or fail to produce diffraction under a high-resolution X-ray.

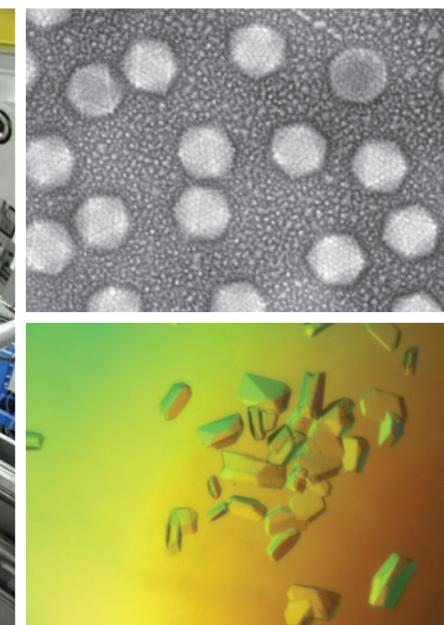
Fischetti and colleagues are upgrading the GM/CA beamlines to provide smaller and more intense X-ray beams that help scientists create clearer images from their crystals. Once the upgrade is completed, Nemerow and Reddy can continue to complete their map of the human adenovirus, so that one day a seasonal nuisance may become a powerful tool for human health. ❁

ADENOVIRUS FACTS

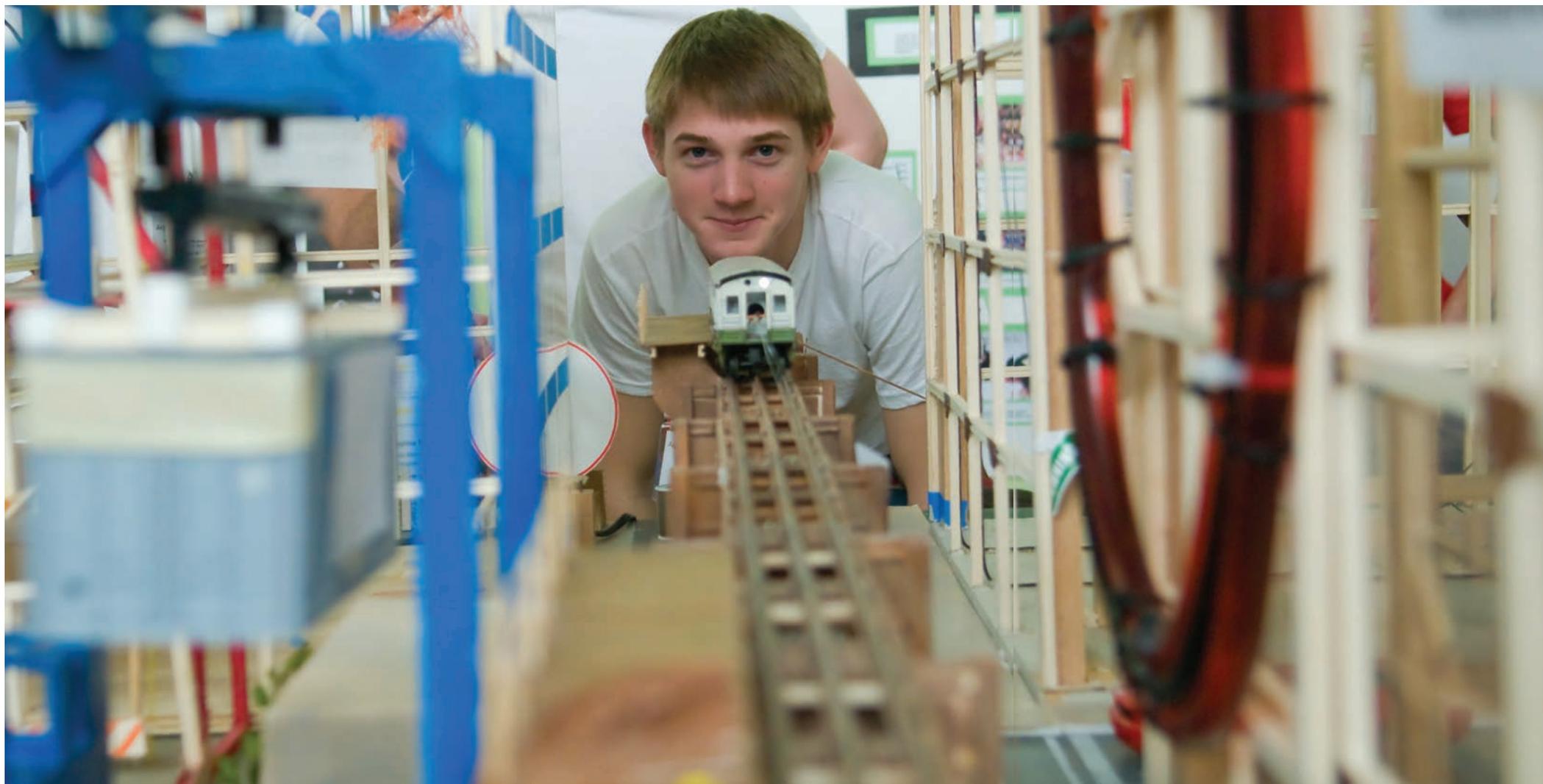
- » Adenoviruses are resistant to cleaning agents and adverse pH conditions.
- » Unlike viruses like HIV, they can survive outside the body.
- » Adenoviruses can cause respiratory illness, ranging from the common cold to pneumonia, croup, and bronchitis.
- » Adenoviruses spread from person to person through the air (sneezing or coughing), by particles left on objects, and by personal contact.
- » Good ways to prevent adenovirus infection include washing hands; covering sneezes; avoiding touching your eyes, nose, and mouth; and staying home from work and school when you are sick.



Robert Fischetti (left), Glen Nemerow (center), and Vijay Reddy load samples at the Advanced Photon Source.



This research is funded by the National Cancer Institute and the National Institute of General Medical Sciences. The Advanced Photon Source is supported by the Department of Energy’s Office of Science.



“For many of my students, field trips are a luxury they cannot afford. After our visit, virtually all of the kids wanted to be the scientists behind the technology. It was great to see so much enthusiasm and to reinforce what we were learning in the classroom and how it applies in the real world.”

— Kevin Hooper, science teacher at Officer Donald J. Marquez School



Fermi’s Footsteps: Education at Argonne

INTRODUCTION TO EDUCATIONAL OPPORTUNITIES AT ARGONNE

Gretchen Anderson’s middle school students saw a lot of cool things when they came to Argonne; they pedaled on a bike to power a light bulb and watched a rubber ball shatter on the floor after a dip in liquid nitrogen. “But

the best part was after the field trip,” Anderson said, “when Argonne employees came to talk with my students about how they overcame obstacles to get where they are today. My students needed to hear this. It made them see

that pursuing a career in science is not just a dream, but a reality.” Argonne offers many excellent opportunities for students in the areas of basic science, energy, environmental management, and national security.

Since Argonne is a multidisciplinary research lab, it can offer science and engineering education programs for teachers and students in physics, chemistry, life sciences, advanced computing, and engineering.

Modern challenges require embracing issues that may span multiple science subjects, rather than the traditional approach of dividing and assigning tasks between discrete disciplines.

Argonne uses an interdisciplinary approach using diverse teams and resources. This arrangement is

fundamental to the design and research approach of the national labs—but it’s also been embraced by education in recent years. That puts the lab in an excellent position to enrich community education; this approach to challenges is highly appropriate for educating tomorrow’s scientists.

> > > *continued*

For more information, visit the Educational Programs website at www.dep.anl.gov, including an updated calendar of events and programs.

Argonne has well-developed education programs directed toward middle school, high school, and undergraduate students, as well as postdoctoral appointments and visiting faculty. More than 3,000 students come to Argonne every year through field trips, single-day events, and other opportunities.

Educational Programs has a

wide variety of offerings. Popular events include Introduce a Girl to Engineering Day, the Rube Goldberg Machine Contest, the Science Careers in Search of Women Conference, and the Middle School Science Bowl, as well as the Undergraduate and Postdoctoral Symposia. Programs and resources for teachers include

the NEWTON Ask a Scientist Program, educational field trips, and teacher workshops and classes. For example, in 2011 the department launched a program for high school students to design and conduct their own research with the guidance of their teachers and Argonne scientists.

For older students, the Visiting Faculty Program at Argonne provides real-world research opportunities for faculty and students from colleges and universities with limited facilities and underrepresented populations. Educational Programs also manages the Indian Education Renewable Energy Challenge (supported

by the Department of Interior's Office of Indian Energy and Economic Development), which is an opportunity for students and teachers to learn about green and renewable energy technology that tribes can use to promote economic and energy independence.

Other resources include access to community outreach and the

opportunity to apply for college internships and research aide positions. Individual researchers also work with Educational Programs to organize research-based opportunities in their own areas.

For more information on any of Argonne's programs, visit the Educational Programs website at www.dep.anl.gov.



A SUSTAINABLE LAB

Argonne has committed to reducing the lab's energy use by 30% by 2015, plus similar goals for greenhouse gases, water use, and pollution.

Two creative ways the lab is greening the campus:



1. GONE GEOTHERMAL Installed in 2012, the geothermal system at the Argonne Information Center saves \$4,000 in heating costs per year and 53 tons of greenhouse gas emissions. Geothermal heating and cooling uses the constant 55°F temperature of the earth to heat and cool buildings. Your fridge actually works by removing heat from the air inside, not by cooling it down. Geothermal works the same way, using pipes of liquid refrigerant that loop deep underground. In summer, the liquid absorbs heat from the air in the Information Center and then releases it as it goes underground. In winter, the liquid picks up heat from the ground and brings it to the surface, where blowers circulate air past the hot pipes and send the warmed air into the building. The pipes below the Information Center go 600 feet underground.

2. SUSTAINABLE STREETLIGHTS Hybrid solar- and wind-powered streetlights, which are completely off the power grid, adorn Argonne sidewalks. A small solar panel and wind turbine powers the LED light atop the fixture, which has batteries to store energy for up to three days without sun or wind.

BY THE NUMBERS

- 9 new all-electric vehicles onsite
- 53% of trash diverted to recycling and reuse
- 75 kilowatt solar array installed this year
- 120 bikes for employees onsite
- 29,000,000 gallons of water saved per year

READ MORE AT
BLOGS.ANL.GOV/GREENLAB



COMING TO CAMPUS

Get a sneak peek at the new buildings sprouting on Argonne's campus as part of its ongoing modernization plan.

THE ENERGY SCIENCES BUILDING

Argonne's new Energy Sciences Building will provide the 21st century scientific infrastructure to attack challenges in sustainable energy. The \$95 million multi-story building will be approximately 160,000 square feet and accommodate an estimated 230 employees.



The building, which broke ground last summer, is designed to bring together scientists in different fields that normally work in separate buildings. In the ESB, catalysis chemists will rub elbows with specialists in magnetic phenomena and materials scientists with transportation engineers. This is the kind of interdisciplinary space that Argonne hopes will help spark revolutions in every field.

Research at the Energy Sciences Building will focus on five central themes: discovery synthesis for designing new materials; bio-inspired nanoscience, which tries to learn from nature to more efficiently harness the power of the sun; catalysis to make reactions faster and better (see page 42); fuel cells, which are a more efficient alternative to fossil fuel combustion; and electrical energy storage, which pursues better batteries.

Groundbreaking: **June 3, 2011**
Building move-in: **Summer 2013**
Construction jobs created: **2,000**

THE ADVANCED PROTEIN CRYSTALLIZATION FACILITY

The State of Illinois is providing funding to help build a special lab, attached to the Advanced Photon Source, where scientists can prep proteins for X-ray scrutiny at the synchrotron.

Protein crystallography is one of the most important tools for drug and vaccine developers, who use the technology to discover the molecular mechanisms of disease in order to design better cures (see page 38). But crystallizing proteins is time-consuming and often frustrating. For every 100 attempts, only one or two usable crystals typically form. "We've designed this facility to shorten the time it takes from producing a protein to making viable crystals from it," said Andrzej Joachimiak, who heads the Midwest Center for Structural Genomics. Scientists at the facility will use robotics to accelerate the production, purification, and crystallization of the proteins.



Construction of the Apcf is expected to create 825 new Illinois jobs and \$25 million in personal income. After opening, the facility is expected to draw another \$110 million for research activities over a five-year period, create 550 new jobs, and add \$52 million to the Illinois economy annually.

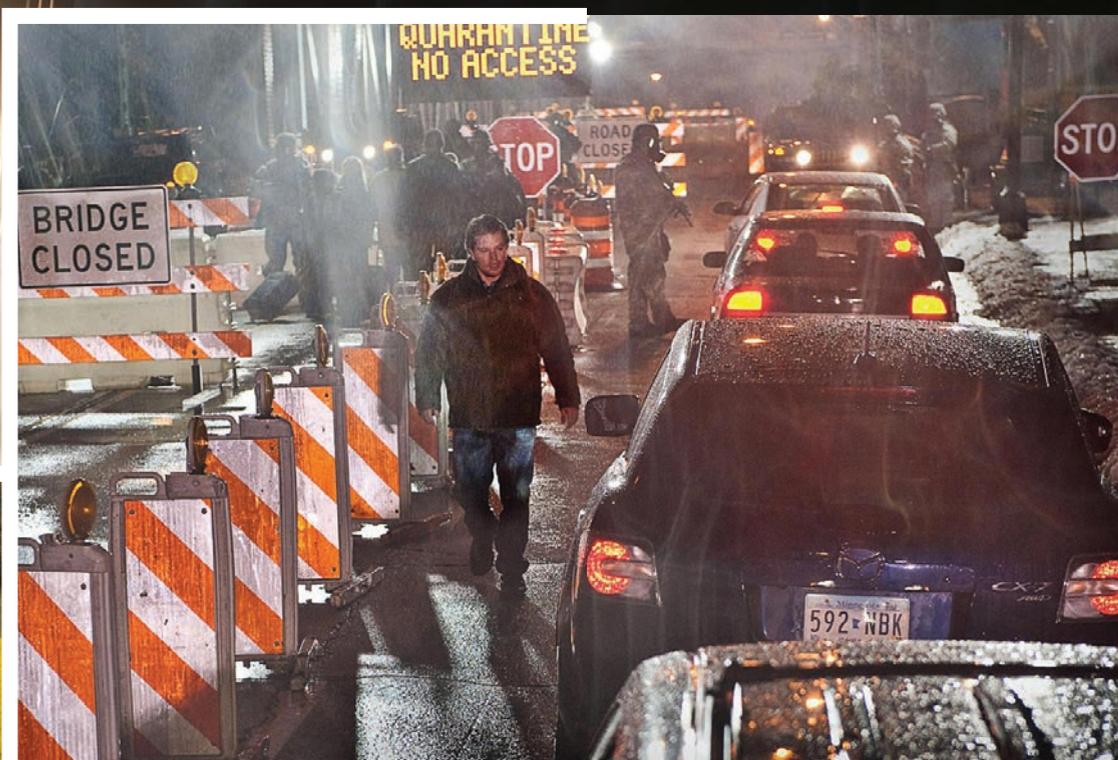
Groundbreaking: **August 30, 2011**
Building move-in: **Fall 2014**
Construction jobs created: **825**

SCIENCE BEHIND THE FICTION

EXAMINES **CONTAGION** [2011]

By Susheela Bhat

Science Behind the Fiction critiques the science portrayed in popular films and literature. Today Argonne emergency planning experts review “Contagion,” the hit movie directed by Steven Soderbergh, which follows the spread of a killer virus in modern-day society.



Sure, a killer virus set on destroying humanity makes a good pitch for a movie. But whether the audience is on the edge of their seats or rolling in the aisles depends entirely on how the movie balances fact and science fiction. 2011’s *Contagion*, however, proved that a thriller can be creative without compromising scientific integrity.

emergency response to an outbreak of the pandemic H1N1 influenza virus.

“With H1N1, people may have gotten a false sense of security because it was so mild. Some thought the CDC overreacted, but you never know what a virus like this can do. If a new virus attacks, we have no immunity.”

Ed Tanzman, who leads the Center for Integrated Emergency Preparedness at Argonne, thought the film exaggerated a few things, such as how quickly they replicated the vaccine. But, he says, “*Contagion* was a pretty accurate depiction of how public health officials would react in real life if a pandemic virus hit their cities.”

He says the film also did justice to the hunt for Patient Zero and the process of looking for the cure, without hyping it up into a modern-day witch hunt.

According to Walsh, “if you can figure out the source, you can figure out where the virus came from. This is something practiced in everyday epidemiology—they always want the source.”

Before they can make a vaccine, researchers need to figure out how the virus itself works. First, they need to grow the virus and observe how it kills its host cells; then they can move on to finding out how to stop it. The actors in *Contagion* portrayed the part of researchers without artifice, Walsh thought, and used the correct language of epidemiology without falling back on the tired stereotypes of science and scientists.

Contagion also demonstrated how a deadly virus can overcome the best containment efforts. Dr. Erin Mears (Kate Winslet) is infected by “fomites,” or inanimate objects (like clothing or hair) that can host infectious organisms long enough

for them to transfer from one person to another. This may have made you leave the theater with the urge to sterilize everything—but it also highlighted how challenging virus containment can be, particularly if it’s an unknown type. (Perhaps it also made you want to wash your hands; if so, all the better—the CDC touts this as a top method of preventing transmission of both viruses and bacteria.)

Tanzman was also struck by how poignantly the movie captured the nature of humanity in the face of such a horrific doomsday scenario. In the movie, Mitch Emhoff’s (Matt Damon) teenage daughter struggles to keep a relationship with her boyfriend, even though they are forbidden from seeing each other while the virus runs its course. Her frustration with having her life put on hold, Tanzman said, reflected how most people would react in that situation.

During a prolonged pandemic, it’s likely that many aspects of society would break down, especially as resources dwindled and basic necessities disappeared. But with the help of experts like Argonne’s Dan Walsh and Ed Tanzman, cities like Chicago can run emergency drills to prepare for the worst-case scenarios. (Turn to page 14 for more.)

“What I took away from that movie, apart from its excellent attention to detail,” Tanzman said, “was that it did an outstanding job of showing the heroism of people in government and public health.

If put in a situation like this in real life, I believe many of them would do the same things.” ❁

Want to get
your news at
99.999% the
speed of light?



You don't have to wait for the next issue of *Argonne Now* to get your daily dose of science and technology.

Follow us online:



Visit our website
www.anl.gov



Follow us on Twitter
twitter.com/argonne



Become a fan on Facebook
facebook.com/argonne



Sign up for our monthly e-newsletter
www.anl.gov/subscribe



Watch science videos
youtube.com/argonnenationallab



See science photos
flickr.com/argonne

www.anl.gov

twitter.com/argonne

facebook.com/argonne

www.anl.gov/subscribe

youtube.com/argonnenationallab

flickr.com/argonne

relatedlinks

- 9 "New Institute to Study Molecular Engineering"
More about the Institute for Molecular Engineering at molecularengineering.uchicago.edu
- 14 "City of Chicago Won't Sweat the Flu"
Watch the video at <http://www.anl.gov/videos/chicago-department-public-health-influenza-drill>
- 20 "The Minimal Microbe"
More about KBase at kbase.science.energy.gov
- 22 "A Natural Solution for Transportation"
More about GREET at greet.es.anl.gov
- 24 "SHARP Could Shave Millions off Nuclear Reactor Design Costs"
More about SHARP at www.ne.anl.gov
- 26 "Introducing Mira"
More about Mira at alcf.anl.gov/mira
- 32 "The Search for the Superbattery"
More on Argonne's energy storage research at www.anl.gov/energy/batteries-and-energy-storage
- 38 "Inside the Advanced Photon Source"
More about the APS at www.aps.anl.gov
- 42 "7 Things You May Not Know About Catalysis"
More about the Advanced Photon Source: www.aps.anl.gov
More about the Electron Microscopy Center: www.emc.anl.gov
More about the Argonne Leadership Computing Facility: www.alcf.anl.gov
- 50 "Argonne in the Marketplace"
More Argonne technologies are available at www.anl.gov/technology
- 52 "The Secret Lives of Nuclear Scientists"
More Clever Apes at www.wbez.org/cleverapes
- 54 "Chasing a Common Cold Virus"
More about GM/CA at www.gmca.anl.gov
- 56 "Fermi's Footsteps"
More about Argonne's education programs at www.dep.anl.gov
- 60 "A Sustainable Lab"
More about Argonne's sustainability programs at www.blogs.anl.gov/greenlab

Sign up to make sure you get
your copy of Argonne Now!
www.anl.gov/subscribe

ask a SCIENTIST

DAN ABRAHAM,
MATERIALS SCIENTIST
ANDY JANSEN,
CHEMICAL ENGINEER

I heard I can make my battery last longer if I let it run out before I charge it. Is that true?



ABRAHAM:

No, not for lithium-ion batteries, which make up the majority of cell phone and laptop batteries these days. This myth is a holdover from older kinds of batteries, like nickel-cadmium batteries, which do benefit from being fully discharged. But that's not necessary for lithium-ion batteries.



JANSEN:

If you want to extend your battery's life, the best way to do that is to keep it from getting too hot. It will drastically shorten the battery's cycle and calendar life if you run it hot.

Put your hand on your laptop battery. It's already hot, right? The battery has to deal with the heat from the processor in your computer, which is like a little furnace; it runs near 120°F. So the less additional heat it has to deal with, the better.

That means even though it's called a laptop, don't keep your laptop on your lap—put it on a hard surface so that the air intake and fans aren't blocked. And of course, don't leave any device with a lithium-ion battery in direct sunlight, in a car, or anywhere else where the temperature can get up over 80°F. Don't put it in a freezer or cold car, either, because the electrolyte can freeze, crystallize, and punch holes in the delicate separator. It's like what happens to meat that gets freezer burn and turns to mush; the same thing happens to a battery.



ABRAHAM:

Interestingly, running at high temperatures actually improves the performance of the battery in the short-term—but over the long run, it will make your performance degrade faster. High temperatures are usually bad for longevity. In fact, when we're testing batteries here at the lab, we accelerate the aging of the battery (in order to simulate years and years of use) by cycling it in a hot chamber, which is typically held at 130°F.

DO YOU HAVE A QUESTION YOU'VE ALWAYS WANTED TO ASK A SCIENTIST? SEND IT TO ARGONNENOW@ANL.GOV.

Science Haiku

SEE YOUR HAIKU IN THE NEXT MAGAZINE! The haiku contest is open to all. You may submit up to three in the traditional English format (one line with 5 syllables, one with 7 syllables, and another with 5, for a total of 17 syllables) covering any aspect of science or engineering. Send entries to haiku@anl.gov.

Using CERN's email
This haiku is submitted
Before I write it...

— William Elias

Einstein taught us this:
If time flies like an arrow,
The arrow is bent.

— Dave Baurac

Muon, gluon, quark,
Lepton, hadron, boson, *sigh.*
Can't they name them Fred?

— Constance Vanni

Haiku Syllables()
if (not line two) return five;
else return seven;

— Amanda Wagner



ARGONNE **INNOW**

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439 USA
www.anl.gov

Non-profit Org
US Postage Paid
Lemont, Illinois
Permit No. 87

Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.



U.S. DEPARTMENT OF
ENERGY

Argonne 
NATIONAL LABORATORY

These “fish” are actually carbon particles made out of olive oil, which work as an ingredient in lithium-ion batteries.

By Vilas Pol