Science & Technology at the Ames Laboratory

inquiry

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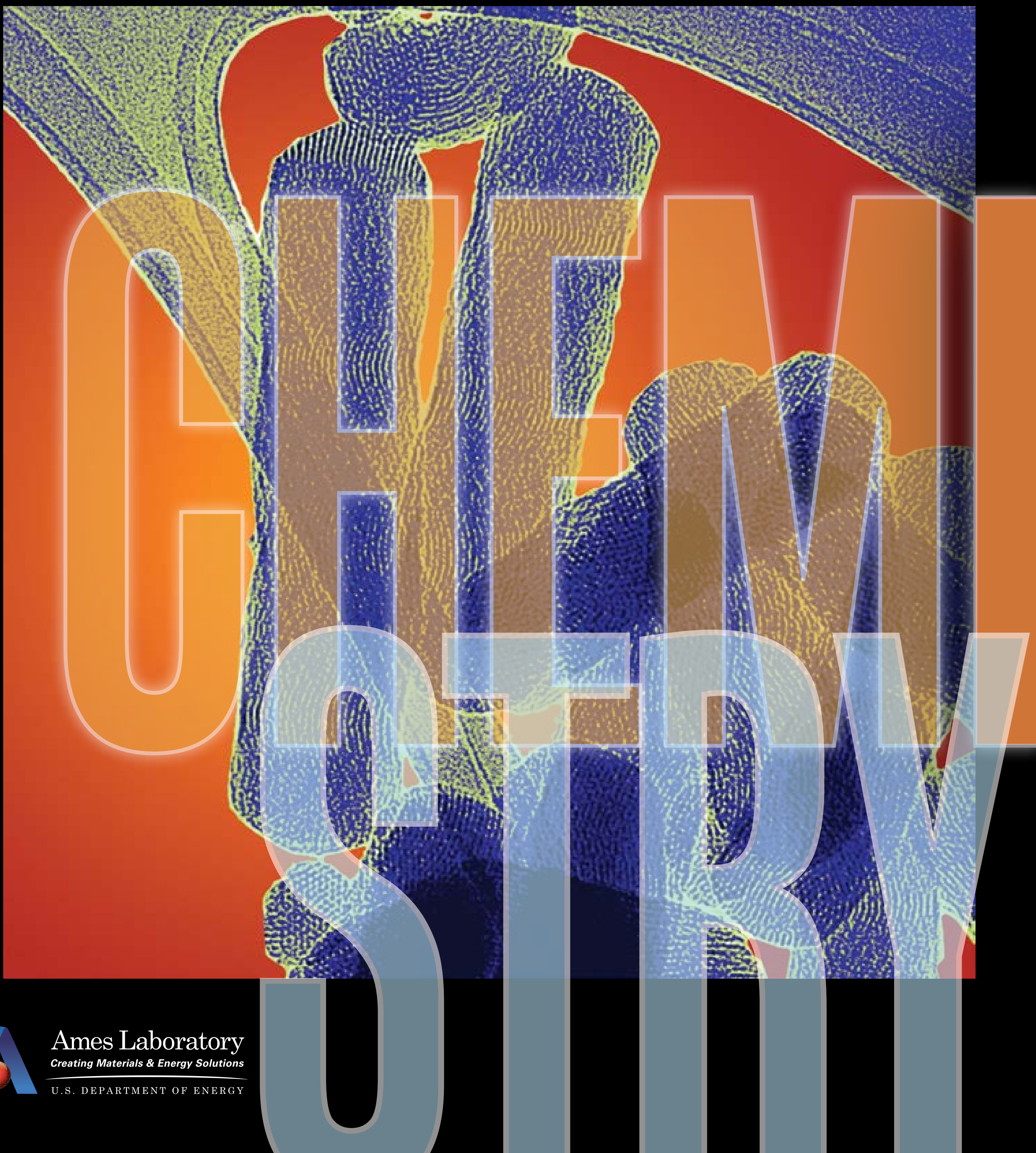
Issue 2

SOLVING THE PLANT PUZZLE • CATALYSTS FOR CHANGE

CUTTING-EDGE ANALYSIS • BACKING A BIG IDEA



Ames Laboratory
Creating Materials & Energy Solutions
U.S. DEPARTMENT OF ENERGY

inquiry

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Ames Laboratory is a U.S. Department of Energy national laboratory seeking solutions to energy-related problems through the exploration of chemical, engineering, materials and mathematical sciences, and physics. Established in the 1940s with the successful development of the most efficient process to produce high-purity uranium metal for atomic energy, Ames Laboratory now pursues much broader priorities than the materials research that has given the Lab international credibility. Responding to issues of national concern, Ames Laboratory scientists are actively involved in innovative research, science education programs, the development of applied technologies and the quick transfer of such technologies to industry. Uniquely integrated within a university environment, the Lab stimulates creative thought and encourages scientific discovery, providing solutions to complex problems and educating and training tomorrow's scientific talent.

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U.S. DEPARTMENT OF ENERGY | Office of Science

From the Director

There's Chemistry in Our Chemistry

Chemistry, broadly defined, is the science of change. Chemists study matter to identify its components and determine the properties and ways in which those components interact, combine and change. They then use their understanding of those processes to form new substances.

Chemistry can also mean that special connection between two people or a group of people. Casting directors strive for that type of chemistry when pairing the leading actors for a motion picture or stage production. Sports fans look for a similar "spark" between a quarterback and his favorite receiver or a cagey point guard who can dish out a no-look pass to the big man for a thundering slam dunk.

As you'd expect, Ames Laboratory research involves a lot of the first type of chemistry and it's the cornerstone of our Division of Chemical and Biological Sciences. As you'll discover in the articles in this issue of Inquiry, our chemists are designing new catalysts to power chemical reactions without the need for powerful (and possibly toxic) solvents or large inputs of energy (see page 6). They're also looking at the chemical processes in plants and developing non-destructive techniques to analyze plant material as it grows in hopes of more efficiently harnessing the energy in biomass (page10).

Others are using state-of-the-art dynamic nuclear polarization (DNP) solid-state nuclear magnetic resonance (NMR) spectroscopy to take a look at molecular structures of materials at unprecedented resolution (page 13). There's also a group studying the big idea of how to mine the energy that winds up in landfills, particularly in the form of plastics (page 16). One of the biggest hurdles is that the plastic is mixed in with other materials, requiring a strategy to chemically convert that mixed waste stream into something useable.

But there's plenty of the second type of chemistry at the Ames Laboratory as well. From the beginning, Ames Laboratory has fostered a collaborative environment that brings together the synthesis, characterization and theoretical aspects of research projects. Experimentalists develop the materials, analytical researchers provide the necessary measurements and theorists model what's occurring. The model in turn provides a suggested roadmap for additional experimentation and characterization.

> From the beginning, Ames Laboratory has fostered a collaborative environment that brings together the synthesis, characterization and theoretical aspects of research projects.

Ames Laboratory also has great chemistry with its contractor, Iowa State University. As the only one of DOE's 17 national laboratories physically located on a university campus, Ames Laboratory can leverage the resources – personnel, equipment and facilities – of Iowa State and vice versa. Nowhere is this chemistry more evident than the new Sensitive Instrument Facility that will formally open for operation in May 2016 (see page 5).

Through cooperative efforts, the SIF was equipped with cutting-edge electron microscopy equipment that will benefit both Ames Laboratory and Iowa State researchers. The final piece of equipment, a $3.5 million aberration-corrected scanning transmission electron microscope, just arrived and will be installed in January. Everyone involved in the project is anxiously awaiting the boost this facility collectively provides us.

Lastly, there's a wonderful rapport that's created through our ongoing DOE-sponsored internship programs. Through the Science Undergraduate Laboratory Internships (SULI), Visiting Faculty Program (VFP) and Community College Internships (CCI) programs, students and faculty participate in research projects with Ames Laboratory scientist mentors. While the benefits to these students are obvious, our researchers also find the experiences rewarding (see page 18).

Thanks and enjoy learning about the chemistry that makes Ames Laboratory what it is.

Adam Schwartz, Director

Awards

Fidler named LANL Director's Fellow

Andrew Fidler

The awards for research excellence just keep stacking up for Andrew Fidler, former Science Undergraduate Laboratory Internship (SULI) program intern at Ames Laboratory.

Fidler's latest award comes from Los Alamos National Laboratory (LANL), the Department of Energy national laboratory where he's currently serving as a postdoctoral fellow. Fidler was named one of LANL's Director's Fellows. Director's Fellows collaborate with LANL scientists and engineers on staff-initiated research. Award selections are based on academic and research accomplishments and the strength and potential impact of the proposed research.

Cassie Dewey, Sallie Spencer and Sarah Morris-Benevides with some of the products that helped Ames Lab earn the DOE Greenbuy Silver Award (center).

Laboratory receives GreenBuy Silver Award

Ames Laboratory recently met one of the 2014 Environmental Management System Steering Committee (EMSSC) goals by winning the DOE GreenBuy Program Silver Award for Sustainable Acquisitions. The Laboratory was one of four laboratories to earn an award from the GreenBuy Program.

To achieve the Silver Award, sites must meet the recycled content or energy savings requirements for a minimum of six products in at least three product categories. In the construction category, Ames Laboratory met 100 percent of the requirements for carpet and flooring materials. Toilet tissue purchases met the requirements within the custodial category. Three of the four office category products purchased (binders, copy paper and servers) met 100 percent of the requirements, while 97 percent of office furniture met the goals of the program.

Todd Zdorkowski (left) and Deb Covey present Ames Laboratory Director Adam Schwartz with the Federal Laboratory Consortium for Techology Transfer Mid-Continent Region Outstanding Laboratory Award. Zdorkowski received the award on behalf of the Laboratory at the FLC's Mid-Continent Region annual meeting on Aug. 26.

Ames Lab named FLC Outstanding Laboratory

Ames Laboratory was named Outstanding Laboratory by the Federal Laboratory Consortium for Technology Transfer Midwest Region. The award is presented to the management of a Mid-Continent member laboratory or facility that has provided exceptional support and encouragement to the transfer of federal technologies to the private sector. Such support and encouragement must have provided tangible benefit to the private sector and to the general public.

Ames Laboratory's Associate Director for Sponsored Research Debra Covey nominated the Lab for the award, based in large part on the work of the Critical Materials Institute.

Outstanding Technical Paper

Ames Laboratory graduate student Stephanie Choquette and scientist Iver Anderson received the 2015 Howard I. Sanderow Outstanding Technical Paper Award from the Metal Powder Industries Federation and its Technical Board.

Thirty-two papers from the POWDERMET2015 conference, held in May in San Diego, were evaluated for final selection. Choquette and Anderson's paper, "Liquid-Phase Diffusion Bonding: Temperature Effects and Solute Redistribution in High Temperature Lead-Free Composite Solders," was selected as the top paper from that group.

Iver Anderson and Stephanie Choquette

Nearly Operational

After more than a year of construction, Ames Laboratory's new Sensitive Instrument Facility is close to being operational. The wet and dry preparation labs have been completed and state-of-the-art microscopy equipment has been installed. The focused-ion beam microscope is currently operational and other pieces are being calibrated and tested. A grand opening of the facility is being planned for May 2016.

The Sensitive Instrument Facility (SIF) is Ames Laboratory's first new research building in 60 years.

Microscopy equipment began arriving in October. Here, the focused-ion beam microscope is carefully unloaded.

The SIF lobby features seating outside the two offices for operational staff, shown in the background.

The building has sample preparation areas for both wet and dry samples, along with a separate instrument repair area.

The lobby is decorated with artwork showing microscopy images submitted as part of a competition.

This transmission electron microscope was the lone piece of existing equipment that was transferred to the SIF.

Collaboration Equation:

Ames Lab Scientists Strengthen Research Through Teamwork

Marek Pruski

Aaron Sadow

Theresa Windus

Igor Slowing

By Laura Millsaps

These days, the fictional stereotype of the isolated and misunderstood scientist toiling alone in his or her lab could not be further from the truth. With scientific disciplines both widely diversified and highly specific, it takes a team of researchers to integrate those disciplines into a unified research goal.

At the Ames Laboratory's Chemical and Biological Sciences Division, a team of scientists advance the frontiers of catalysis—the acceleration of chemical reactions—through the use of three-dimensional nano-particles.

The beginnings of the 3D catalysis project in 2002 was sparked by nuclear magnetic resonance spectroscopy expert Marek Pruski and the late Ames Laboratory scientist Victor Shang-Yi Lin. Together they wanted to pair the development of three-dimensional scaffolds for catalysis designed by Lin with the best possible NMR spectroscopy methods for characterizing them developed by Pruski. "It was a natural symbiotic relationship," remembers Pruski.

And just like reactions are spoken of in the language of chemical equations, over time the interactions of scientists in the Ames Laboratory's catalysis program have created an equation of their own, where the right balance of experiment, characterization and theory adds up to something more than the sum of their individual parts.

Chemist$_2$

"We're creating fundamental and unique chemical functions for important transformations."

– Aaron Sadow

Ames Laboratory scientist Aaron Sadow studies chemical reactions that can be manipulated and controlled toward a specific purpose. With an interest in organometallics, he hunts for catalysts that can be stabilized and made more efficient for petrochemical, biorenewable, and shale-gas chemical processes.

"We're creating fundamental and unique chemical functions for important transformations," said Sadow.

He collaborates with scientist Igor Slowing, who specializes in developing mesoporous nanoparticles from silica and other materials that provide a platform for these chemical reactions to take place.

While the creation of new and useful catalysts is a goal, so is understanding specifically how these three-dimensional catalytic structures function the way they do.

"When we attach these catalysts to materials, we're changing how they perform. We're comparing heterogeneous or non-soluble forms to soluble forms of the catalyst, the effects of immobilizing them in these support systems, and how they work differently," said Sadow.

"We're trying to understand how the structure and design of these platforms affect the catalytic processes," said Slowing.

$Chemist_2$ + NMR Spectroscopy + $Theorist_3$ = World-Class Catalysis Research

"The pores in these particles force molecules to move in different ways, and we need to know more about that in order to optimize these catalytic systems to work the most efficiently."

NMR spectroscopy

"Honestly, without Marek we'd be flying blind."

– Aaron Sadow

Marek Pruski's group provides guidance to other project members with the structural insights. To do so, Pruski uses Ames Laboratory's state-of-the-art solid-state NMR instrumentation, including the recently acquired dynamic nuclear polarization (DNP) NMR spectrometer, the first in the nation to be used exclusively for materials science research. Its use represents up to a 300-fold increase in sensitivity and a "transformational" technique in providing information to experimental researchers and theorists.

"No other method of spectroscopy can probe the structure of materials with such atomic-level sensitivity to the local electronic environment," said Pruski. "Until you carry out proper characterization of a catalyst, you can only make educated guesses about what the structure might be. It's one of the unique strengths of this program that we can provide a very thorough characterization of catalysts as we build and use them."

That's helped guide experimentalists Sadow and Slowing work towards common research goals, refining the designs of both the mesoporous structures and the catalysts themselves.

"Honestly, without Marek we'd be flying blind," said Sadow.

"We of course want these systems to work well, to be useful, but we also want to understand how they work," said Pruski. "If we can achieve that understanding, we can engage in a rational design of catalytic systems rather than rely on serendipity."

$Theorist_3$

"We try to help them figure out what exactly happens in the middle. It's a way of verifying and understanding their experimental results. "

– Theresa Windus

Three theorists have contributed their computational modeling expertise in order to better understand the systems the experimentalists are designing.

One of them, Theresa Windus, an Ames Laboratory associate in chemistry, has provided Sadow with computer models of the reaction mechanisms of the catalysts he and Slowing are building.

"They have their catalyst, and their reactants and end products, but they can't really see the reaction itself occurring. We try to help them figure out what exactly happens in the middle. It's a way of verifying and understanding their experimental results, infrared and NMR spectra," said Windus.

Many times, said Windus, it begins with a dialogue. "They'll ask us to verify some experimental result, and after doing the computations, we'll realize that we're not getting what they think we should. Then we go back to them and ask 'is there another explanation for what's happening?' It becomes a very synergistic information loop."

Additionally, Ames Laboratory associate Jim Evans has provided Igor Slowing kinetic models describing how molecules move within the nanopores of the materials, and Ames Laboratory associate Mark Gordon has contributed to the group with molecular modeling of chemical processes on the surfaces of the materials.

Taken altogether, Sadow considers the contribution of the three an asset to the experimental side.

"I think that you can force systems to behave in certain ways,and ask questions about them in theory that you really cannot ask in an experiment," said Sadow. "That helps us consider different possible pathways to the same result, and which one best describes what's actually happening."

World-class catalysis research

"A single person cannot realistically have all the skills needed to fully interrogate matter. You need many people, many skills."

– Igor Slowing

Ames Laboratory's combination of catalysis, spectroscopy and theoretical experts creates a widely respected research reputation in a field that has far-reaching impact in industrial, environmental and medical applications.

"When I first began my research group's work, I only felt comfortable proposing research that I individually had the skill set to accomplish," Sadow said. "That's always the individual's limitation. With others' contributions, the scope of what kind of problem you can tackle becomes much greater, and that's the great appeal of our research group."

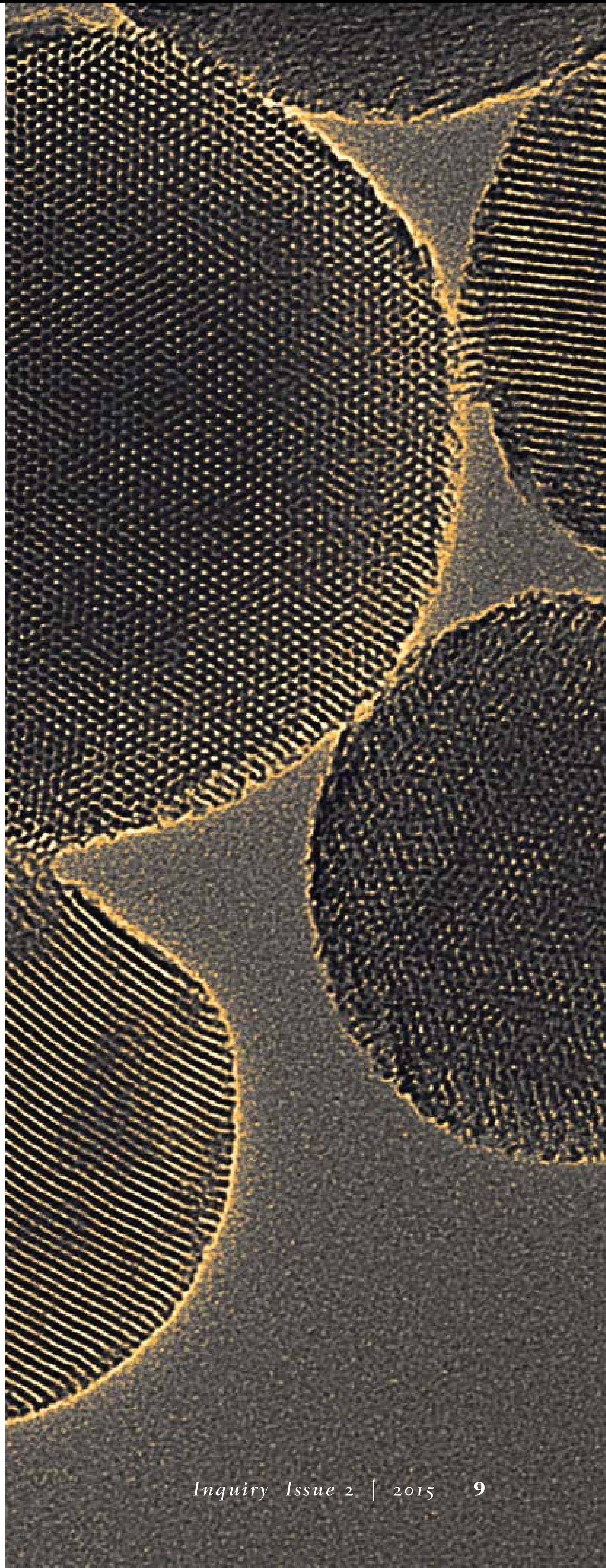
Windus considers it personally gratifying to have impact on disciplines outside her own area of expertise. "Catalysts are a lot of fun," she said. "They are amazing compounds that make perfectly impractical reactions viable, useful and doable, and I enjoy making contributions to applied science."

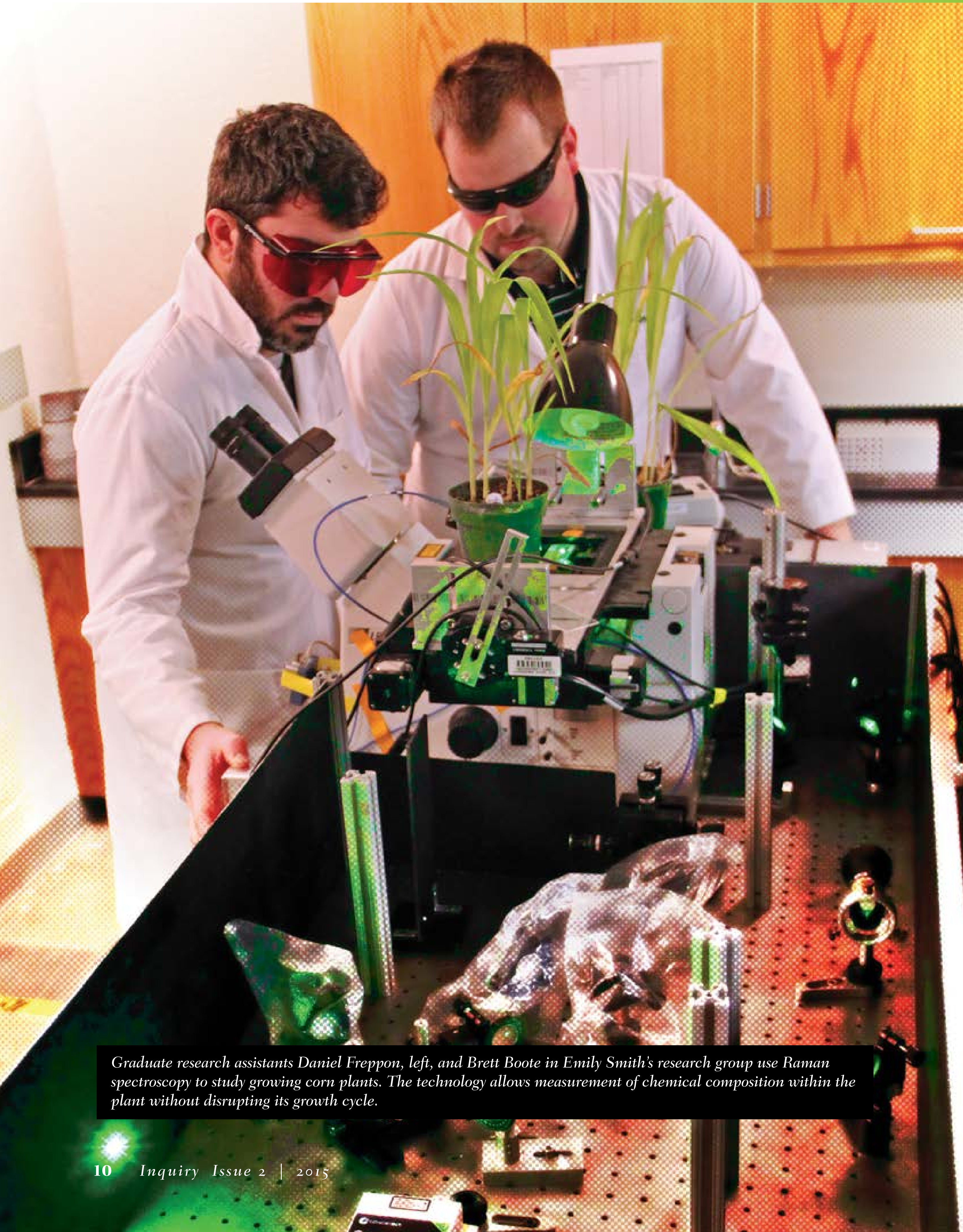
And in a broader sense, Slowing believes collaboration is also fundamental to success in today's research world.

"It's a huge value, the way science is right now. You can try to master as many different things as you can, but a single person cannot realistically have all the skills needed to fully interrogate matter. You need as many different specialists in as many diverse areas as possible to be successful."

According to Pruski, Ames Laboratory has continued to lead in the field of catalysis because of the synergistic efforts of world-class researchers.

"We don't work together just because we all happen to be here in one place. The synergy of this program is truly vital, and real."





Graduate research assistants Daniel Freppon, left, and Brett Boote in Emily Smith's research group use Raman spectroscopy to study growing corn plants. The technology allows measurement of chemical composition within the plant without disrupting its growth cycle.

"we want to visualize …this eloquent dance of molecules in and across the membrane …"

Basil Nikolau,
Director of ISU's Center for Metabolic Biology

Solving the Biomass Puzzle

BY KERRY GIBSON

Biomass holds great promise as a petroleum replacement, but unlocking its true potential remains a puzzle. A group of researchers at Iowa State University and Ames Laboratory hope to develop the pieces of that puzzle to create a clearer picture of what takes place within a plant and how that applies to its downstream uses as biomass.

The $1.8 million, three-year project, funded by the Biological and Environmental Research program within the Department of Energy's Office of Science, brings together a diverse team of Iowa State plant scientists and computational experts, as well as analytical chemists from Ames Laboratory. The group will explore the fundamental ways plants produce and store energy, how to potentially optimize those metabolic processes, and then compile the vast amounts of information collected in an accessible format.

"It's very fundamental science," said Basil Nikolau, director of ISU's Center for Metabolic Biology and one of the principal investigators on the project. "Everyone can easily recognize a plant, but as you use ever more powerful microscopes to look at it in more minute detail, down to the molecular level within individual cells, you lose context of it as a plant. So we're looking for a way to represent these details within the overall context of the plant."

Plants use photosynthesis, a process fundamental for most life forms on Earth, to capture sunlight and convert it to chemicals. But how does that happen?

"We know the initial chemistry involves separating charged particles across a membrane," Nikolau said. "At its core, this project will develop analytical imaging technologies to visualize the organization and dynamics of the membrane that enables this eloquent dance of molecules in and across the membrane to convert sunlight to chemistry."

Though not useful as a biomass source, the team is studying Arabidopsis as a model system. The plant's genome has been mapped and it readily lends itself to study. The group is also studying corn, another plant with a vast amount of genetic background information, and a crop that's important to Iowa and as a potential biofuel source.

"You can grow it in a small space and it grows quickly," Nikolau explained of Arabidopsis, "so you can produce six to eight generations in a year. It's an ideal plant to study, and what we discover is generally applicable to other crops as well."

Specifically, the group is using Arabidopsis plants that have been genetically altered to boost autophagy, a process plants use to survive resource (carbon or nitrogen) limitations.They'll look at how the plants use a vesicle called an autophagosome to conserve biomass and energy to survive the resource deficiencies.

Iowa State University plant scientists (l-r) Eve Syrkin Wurtele, Basil Nikolau and Diane Bassham display plant materials being studied in a campus greenhouse where the plants are grown.

Analysis of the plant material relies on the technical expertise of a cadre of Ames Laboratory researchers. Using techniques such as Raman spectroscopy and stimulated emission depletion (STED) fluorescence lifetime imaging as well as more traditional mass spectroscopic methods, they are able to generate detailed information of not only the chemical makeup within the plant, but also the processes and changes taking place within the living plant throughout its growth cycle.

"Ideally, we want to be able to measure the plant as it's actually growing, without disrupting it or extracting

All involved say the project perfectly melds the strengths of ISU and Ames Laboratory.

material," said Emily Smith, Ames Laboratory scientist and ISU associate professor of chemistry. "That means using imaging techniques that provide exquisite spatial resolution that shows you structures and molecules. You also want to get chemical information, to know exactly what chemical compounds are present. "

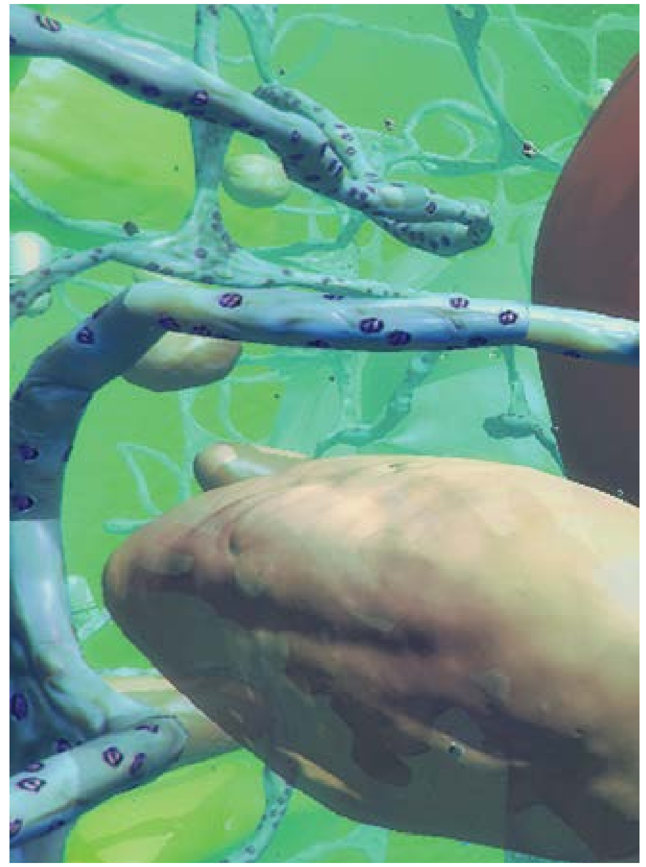
"The STED gives us good spatial resolution so we can look at subcellular structures," Smith continued. "The Raman imaging gives us the chemical analysis so we know, for example, what fatty acids are present."

In addition to these techniques by Smith's group and ISU researcher Jacob Petrich, the team is aided by ISU associate professor of chemistry Art Winter who has developed molecular probes that selectively "light up" or "turn on" certain elements within the cell that can then be captured by the STED imaging. Ames Laboratory scientists Sam Houk and Young-Jin Lee provide additional chemical analysis through advanced mass-spectroscopy methods, and provide a means of validating the images obtained by the other imaging technologies.

"One of the downsides to using the techniques we've developed is that you can get so much information that one person couldn't begin to sort out what's important," Smith said. "That's where the computational techniques developed by Eve Syrkin Wurtele and Diane Bassham come into play to sort out the needle of useful information in the haystack of data to address the particular biological question we're posing."

Wurtele and Bassham, both professors of Genetics, Development and Cell Biology at ISU, use an integrated experimental/biocomputational approach to understand the factors that regulate plant development and composition. That includes an award-winning computer visualization program – yep, a video game – called Meta!Blast. Data can be imported into the program and it provides a visual depiction of what's taking place within the plant at the appropriate cellular or molecular scale.

"The idea is that you have this visual environment that's new to most people and you can do things like scan structures or molecules if you don't understand them, get an explanation of the analytical technologies, and see multiple vantage points," Wurtele said. "The various chemical and biological (analytical) techniques let you create an image of the plant and its molecular components that is at a resolution from a multicellular level, like the surface of a leaf, to the cellular, into the organelles within individual cells, and ultimately the individual molecules."



This image from the Meta!Blast program shows structures within the cells of plant. The program is used to visually represent huge volumes of data collected from living plants to accurately depict what takes place chemically and physically within the plant.

All involved say the project perfectly melds the strengths of ISU and Ames Laboratory.

"In our group, we're all experts in our own domains, but I don't think there's one person who fully understands the other people's technologies," Wurtele said. "The idea behind this is to create a system where the actual data that's obtained at different resolutions and spatial compartments is integrated so that anyone is able to access the data in an understandable form."

"It's a highly collaborative project," Nikolau added, "and a very good fit between the biological and the analytical sides."

"We developed these various analytical techniques for other purposes," Smith concluded. "With this project, we're able to apply them to biological materials. ISU is extremely strong in plant science and Ames Lab has vast analytical expertise, and it's been great to see this synergy develop. Hopefully we can leverage that down the road on future projects."

Higher Speed, More Precision

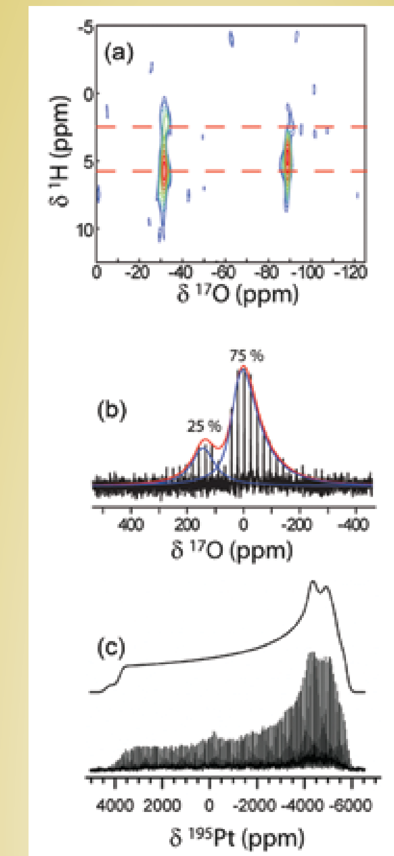
BY BREEHAN GERLEMAN LUCCHESI

In just a little over a year of operation, Ames Laboratory's dynamic nuclear polarization (DNP) solid-state nuclear magnetic resonance (NMR) spectrometer has successfully characterized materials at the atomic scale level with more speed and precision than ever possible before. Spectra for materials important to catalysis, solar energy, and hydrogen storage have helped scientists better understand how these materials work.

Conventional NMR detects the responses of atomic nuclei to direct excitation by radio frequency waves. DNP-NMR offers faster and more detailed spectra over traditional NMR by first exciting unpaired electrons at their microwave resonance frequency and then transferring the resulting spin polarization to the material's nuclei. This additional step results in much stronger signal intensities from these "hyper-polarized" nuclei than is available by conventional means.

The advanced capabilities of DNP-NMR have already made it possible for Ames Laboratory NMR experts to answer questions that were out of reach before.

For example, in a paper in the Journal of the American Chemical Society, Ames Laboratory scientist Marek Pruski and his research team reported on DNP studies of natural abundance ^{17}O in several materials. Oxygen is practically undetectable by conventional NMR due to its



DNP-enhanced ^{17}O (a and b) and ^{195}Pt solid-state NMR spectra (c) of surface species. In (a) a natural abundance ^{1}H-^{17}O HETCOR spectrum of silica surface allowed for the distinction of hydrogen-bonded and non-hydrogen-bonded silanol sites. In (b) natural-abundance ^{17}O NMR enabled, for the first time, the detection of defect sites in MOFs. In (c) ^{195}Pt NMR experiments of surface-bound Pt sites enabled the unambiguous characterization of their binding environment.

Ames Laboratory scientist Marek Pruski, left, and Ames Laboratory postdoc and Spedding Fellow Frédéric Perras stand next to the DNP NMR equipment.

Hardly a week passes where we don't get a contact from other researchers about DNP, and the instrument is operated non-stop ...

Takeshi Kobayashi, left, looks on while Frédéric Perras loads a sample into the DNP NMR equipment.

low natural abundance and quadrupolar nature. "The signal enhancement that DNP provides, allows for detection of ^{17}O without enrichment," said Pruski. "The detection of ^{17}O nuclei was among our key targets early on, because oxygen is one of the most ubiquitous elements in materials."

Frédéric Perras, Pruski's colleague and Ames Laboratory's Spedding Postdoctoral Fellow, used DNP to hyper-polarize ^{1}H nuclei, and subsequently transferred ^{1}H polarization to ^{17}O, cleverly using a scheme called PRESTO, which was published over 10 years ago and then nearly forgotten in the NMR community. Perras has since used DNP-enhanced ^{17}O solid-state NMR to characterize mesoporous silica nanoparticles (MSNs) and metal organic frameworks (MOFs) without expensive isotope enrichment (shown in the figures on page 13).

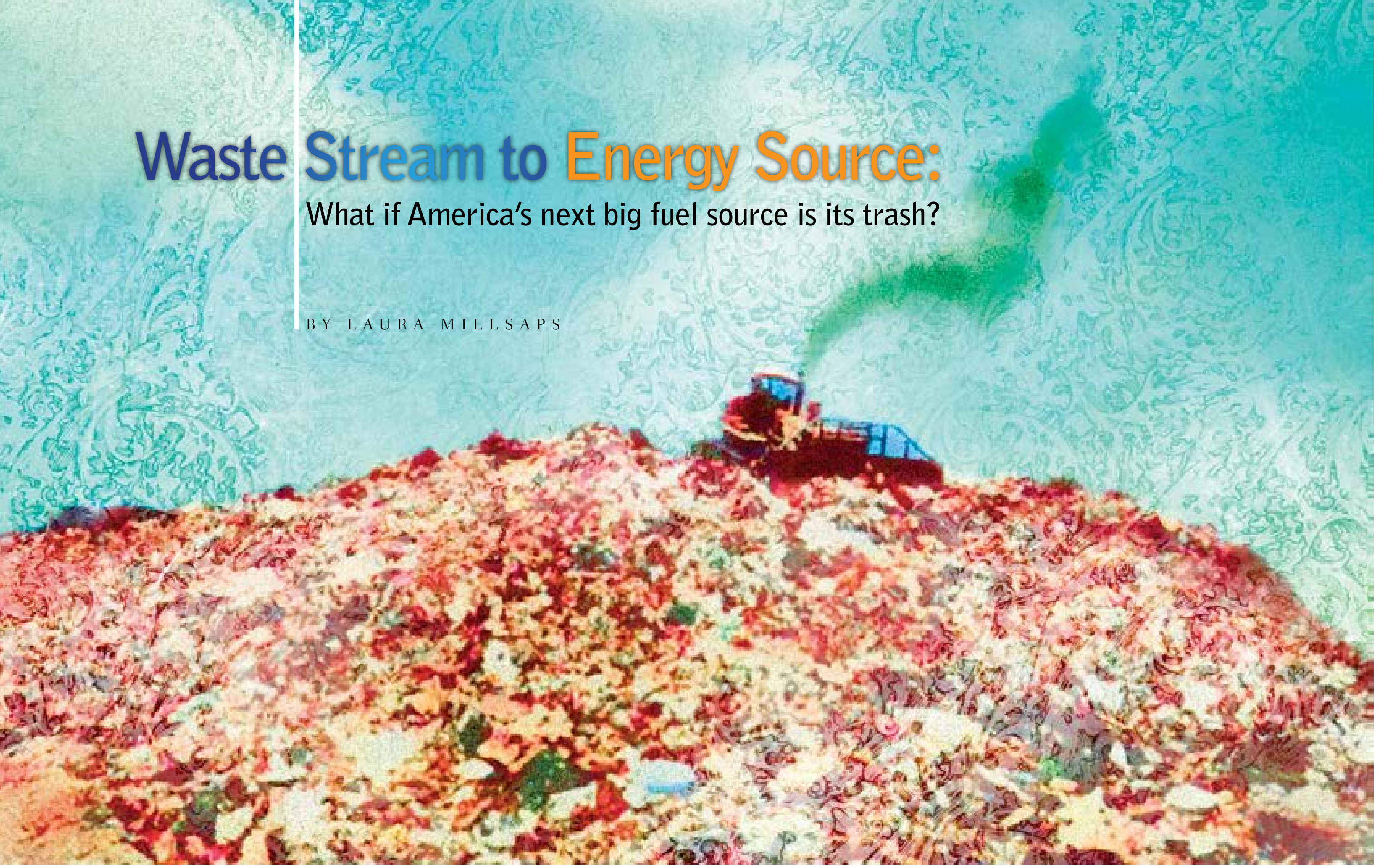
Pruski and his team, which also includes Ames Laboratory scientist Takeshi Kobayashi, use DNP-enhanced spectra of other nuclei, such as ^{15}N, ^{29}Si, ^{27}Al, ^{195}Pt, and ^{207}Pb, to make key characterizations of a variety of other materials prepared at Ames Laboratory.

They collaborate with Aaron Sadow's and Igor Slowing's research groups on the design and testing of new types of supported catalysts, as well as new polarizing agents that may offer even more improvement in DNP measurements. They also work together with Vitalij Pecharsky and co-workers on understanding the solid-state transformations in complex metal hydrides. The 'DNP contingent' has been further strengthened by Aaron Rossini, who recently joined the Ames Laboratory as a faculty scientist. Rossini's interests include DNP characterizations of novel materials as well as DNP method development.

"Hardly a week passes where we don't get a contact from other researchers about DNP, and the instrument is operated practically non-stop," said Pruski. "Our external collaborations include Iowa State University, Argonne National Laboratory, Northwestern University, Washington University, University of Delaware, University of Lille (Lille, France), University of Wisconsin and Purdue University, and the list continues to grow."

One important next step is enhancing the capabilities of DNP by designing new pulse sequences, instrumentation, highly efficient polarizing agents and improved sample formulations, in order to open new doors to even faster, detailed measurements of materials' properties. Pruski's team is engaged in this effort.

"DNP was invented by physicists and then first widely used by researchers to characterize biological systems, but I think many would agree that the primary beneficiaries of DNP are materials scientists and chemists," he said. "The technique is particularly well suited for studying the surfaces of materials. But, it's still early and much work is needed to improve the technique."



Waste Stream to Energy Source:

What if America's next big fuel source is its trash?

BY LAURA MILLSAPS

According to the U.S. Environmental Protection Agency, the United States produced 254 million tons of municipal solid waste in 2013. And though 87 million tons of that material from landfills was diverted through recycling and composting, what if the nation could do better? What if landfills could become local sources of clean energy production? Better yet, what if all waste streams, like those from agricultural, livestock, and food production, could essentially become fuel refineries at a local level?

It's a question being asked by a collaboration of national laboratory researchers who want to create energy conversion technologies designed to mine the carbon out of waste processes that traditionally have been an environmental burden to the planet and a disposal headache for humans.

"The idea of using waste as energy source really isn't new," said Cynthia Jenks, assistant director of Scientific Planning and division director for Chemical and Biological Sciences for Ames Laboratory. "For example, some municipal and regional utilities already burn landfill waste as a source for electrical power. But we think there are better, cleaner and more efficient ways to get at that carbon and use the potential energy from it."

A new concept was born of the Big Ideas Summit, held by the Department of Energy and its national laboratories in 2015. The effort, being co-led by Ames Laboratory and Pacific Northwest National Laboratory, is a collaboration of 12 national laboratories to find new catalytic technologies that can efficiently produce biofuel from waste streams.

The goals are specific. Make the technology as simple as possible, yet adaptable to diverse waste streams. Locate it right at the waste stream source, whether it's a landfill, livestock farm or commercial facility. Make it easy and economical to produce and deliver through the use of modular manufacturing.

> "That's really the 'big idea,'" said Jenks. "Where there is waste, there is energy."

"The idea brings together a lot of overlapping interests: chemical research, applied engineering, modular manufacturing, waste management, agriculture, industry, and energy-sector investors. It's a complex idea with a lot of moving parts, but one that we think will get us a lot closer to accessing the potential energy in these underused resources, and a lot closer to the nation's sustainable energy production goals," said Jenks.

To meet the goal, the participating national laboratories will pool their skills in materials and chemical sciences, high-performance computing, engineering, and applied technology. Ames Laboratory will lend its expertise in catalysis to the project through its Chemical and Biological Sciences Division. Scientists Igor Slowing and Aaron Sadow have already done extensive work in creating catalysts that are able to convert carbons, by placing catalytic agents on high-surface-area nanomaterials. They want to develop processes that make possible the controlled decomposition of waste polymers into useful hydrocarbons.

"A large amount of the waste that goes into landfills is polymers…plastics. These are very carbon rich, very processed materials, and if we were to be able to convert that waste into new, useful compounds or energy, that would make much better use of them," said Sadow. "Right now, we're wasting all that carbon. It's just sitting there in the trash."

Sadow and Slowing will also be applying similar techniques to the conversion of wet sludge and agricultural wastes.

Sadow said the scientific challenges are complex, with a need for chemical reactions that can be highly efficient, operating at low temperature and low pressure. They will also need to be capable of adapting to changes in the raw material feeding them.

"Any waste stream is very mixed, and its composition varies over time," said Sadow. "We can physically sort and then convert, but then there's that separation step. We don't really know how to chemically convert mixtures in general. That is a really big, interesting, fundamental challenge that research hasn't yet tackled, and that's exciting to contemplate."

While the group estimates that these localized biofuel refineries would produce small quantities of biofuel—an average of the equivalent of 125 barrels of oil per day—the collective impact could be staggering. Transforming the available national waste streams into fuels and other useful chemical products could translate to the equivalent of 2.7 billion barrels of oil per year, or 40 percent of the nation's annual crude oil use.

"That's really the 'big idea,'" said Jenks. "Where there is waste, there is energy. We believe that the collective expertise of the national labs, including the chemical research strengths of Ames Laboratory, puts that big idea within reach."

> "A large amount of the waste that goes into landfills is polymers…plastics. These are very carbon rich, very processed materials, and if we were to be able to convert that waste into new, useful compounds or energy, that would make much better use of them. Right now, we're wasting all that carbon. It's just sitting there in the trash."
>
> Aaron Sadow

Chemists Leave Their Mark on Future Scientists

BY STEVE KARSJEN

Eight out of the past 10 years, Ames Laboratory chemist Aaron Sadow has mentored a Science Undergraduate Laboratory Internships (SULI) student. Sometimes the mentorship has been for the 10-week summer program and sometimes for the 16-week semester program. On occasion, he's mentored more than one student at a time.

When asked why he keeps coming back to the SULI program, Sadow, who is also associate professor of chemistry at Iowa State University (ISU), responded, "SULI is an excellent program for everyone involved. Mentors benefit from having the opportunity to help train future scientists to do great science, graduate students benefit from having the opportunity to work with excited undergraduate students, and interns benefit from research opportunities that may result in published research papers that could lead to additional research funding for the mentor's program."

Including Sadow's students, Ames Laboratory scientists featured in this issue of Inquiry have hosted more than 50 students and faculty from 34 universities, colleges and community colleges around the country.

Holding a close second to Sadow's impressive record of commitment to Ames Laboratory's science internship programs is Ames Laboratory scientist and associate professor of chemistry at ISU Javier Vela. But in addition to hosting several SULI students, for the past six years Vela has hosted two Visiting Faculty Program (VFP) teams, which consist of a faculty member and up to two students. With a focus on growing a diverse workforce for the Department of Energy's national laboratories, VFP teams come from institutions historically underrepresented in the research community.

"It is only because of this program that we've have had an opportunity to collaborate with the principal investigators at these institutions," said Vela, who was a 2014 recipient of the Stanley C. Israel Regional Award for Advancing Diversity in Chemical Sciences. "And most of the students we've hosted would never have thought about coming here. They've been able to learn more about our Laboratory, university, city, and state. It's been a good experience all-around."

Javier Grajeda, a SULI intern in 2011, epitomizes the importance of internship programs like VFP that are focused on diversity. Vela met Grajeda, a student at the University of Texas at El Paso (UTEP) at a Society for Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) conference. A discussion of Vela's work in inorganic chemistry piqued Grajeda's interest so he applied for the summer 2011 SULI program. During his short internship, Grajeda co-authored a paper with one of Vela's graduate students, which was published in the journal Chemistry of Materials. In addition to working in his lab, Vela said Grajeda also continued working with scientists at UTEP and then traveled to China to do research. When it was time to apply for graduate school for his Ph.D. in chemistry, Grajeda was accepted at the University of North Carolina at Chapel Hill. At the same time, he was awarded a highly competitive three-year fellowship through the National Science Foundation Graduate Research Fellowship Program. When asked about the key to his success, Grajeda said, "Working under Dr. Vela has had a great impact on my career, and I'm grateful for having been given the opportunity to participate in the SULI program."

> **... everyone wins with the DOE's internship programs ...**
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> Javier Vela, Ames Laboratory scientist

Although he would have preferred to have had Grajeda enter graduate school at Iowa State, Vela takes a long view of the situation and said ultimately "everyone wins with the DOE's internship programs" because they help facilitate the growth of students like Grajeda, who may end up working as scientists at DOE laboratories.

Ames Laboratory scientist Igor Slowing, who has mentored 10 SULI students since 2012, echoes Vela's comments. Slowing said internships offered through SULI, VFP and the Community College Internship (CCI) program are a "good advertisement" for Ames Laboratory. "What we are doing in the DOE's labs is communicated to more people, which in turn helps universities and communities learn more about the DOE and its national labs, which then helps the American taxpayer understand what we're doing with their taxpayer dollars," said Slowing.

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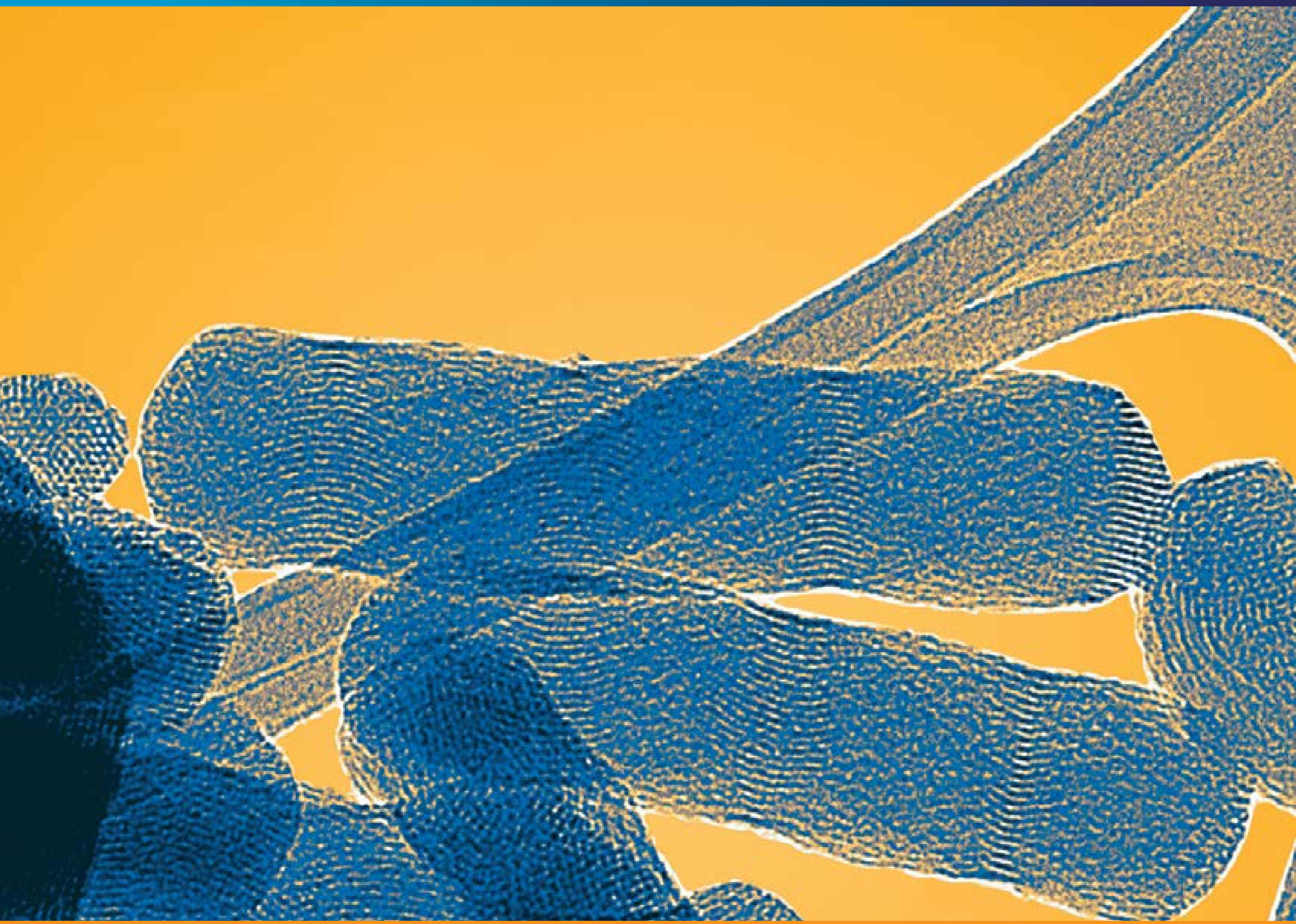

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