NREL
NATIONAL RENEWABLE ENERGY LABORATORY

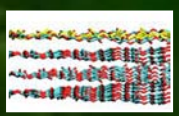
Continuum
MAGAZINE
Clean Energy Innovation at NREL

nrel.gov/continuum

Winter 2012

Deliberate Science

Reinventing
Material Science



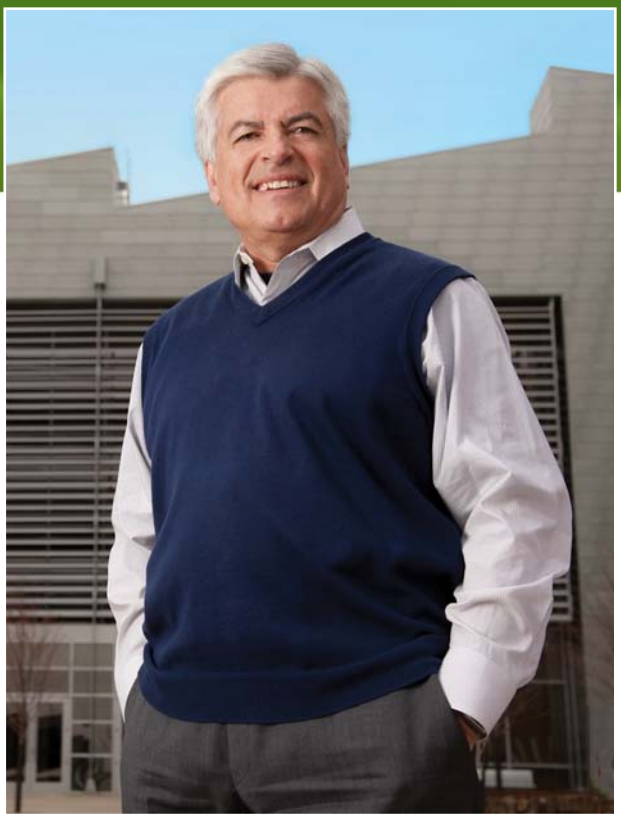
Better Biofuels through
Computational Analysis

Supercomputing
Drives Innovation

NREL is a national laboratory of the U.S. Department of Energy,
Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Dan Says

Producing Game-Changing Innovation to Benefit the Nation, As Fast and Effectively As Possible



Dr. Dan E. Arvizu, Laboratory Director

It's a question almost as old as the scientific method itself: What's the best way to conceive and manage the process of scientific inquiry? On one side are those we might describe as "blue sky" gazers, who value the unlimited potential of basic science. Their philosophy: explore the physics and chemistry of nature, and good science will reward you with unexpected insights — some more profound than you ever could have imagined.

On the other side are the pragmatists among us, who might in turn respond, how can we achieve an end result if we don't first define it, then work steadily toward that goal?

As a scientist and director of the nation's only national laboratory devoted solely to clean energy research and development (R&D), the question of how to most effectively perform our work is one I grapple with every day. The National Renewable Energy Laboratory is renowned as an *applied energy laboratory*. Our purpose is to directly impact the energy industry. While that suggests the results-driven model of science and technology, experience tells us we must employ every tool available to us. What we've learned through more than three decades of successful renewable energy and energy efficiency technology R&D is that there is no inherent dichotomy between pure science and use-driven science. Each works best when both work together.

This approach might best be called "deliberate science." Everything we do at NREL is deliberately focused toward helping the nation reach its clean energy goals. How we get there, however, doesn't come about in a straight line. Rather, it's a complex, dynamic process. The insights we gain through the basic science we perform is essential to our applied technology R&D, and that in turn greatly shapes how the technology moves on to commercialization and deployment in the market.

You'll see how this process guides work in each of our research fields as you read the articles in this, the second issue of *Continuum*.

For the dedicated professionals with whom I'm privileged to work at NREL, this is the best of both worlds. Our highly specialized research teams dive deep to answer the fundamental questions of science. Their colleagues forge those new insights into workable concepts for breakthrough technologies. Teams focused on systems integration, testing, and validation then reduce the risk of new technology to the point where private industry can make the investments needed to commercialize and deploy it.

At NREL we utilize the whole toolkit of science, with a specific, market-relevant use in mind. Deploying valuable new energy technology may always be the overriding end goal. Yet getting there in the most efficient way possible means that there is no bright line where basic science ends, and

continued on page 24

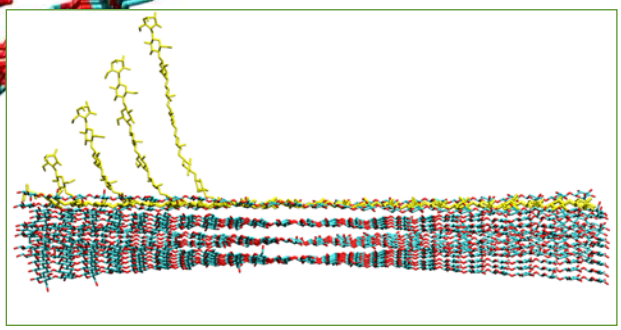
Content

Winter 2012

Features

Articles

Better Biofuels through **Computational Analysis**



Yellow chain in simulation shows stages of pulling a single cellulose chain out of a crystalline cellulose microfibril. The natural twist in the microfibril is evident in the bottom three layers. NREL scientists calculated the thermodynamic barrier that an enzyme must overcome to decrystallize cellulose.

Developing and applying a powerful arsenal of computational tools for producing biofuels.

It's tough to break down woody material into its component sugars—so tough that scientists describe this characteristic as the "recalcitrance of biomass." Making the process even more difficult is the fact that the natural cellulase enzymes that can do the job act very slowly.

This recalcitrance is actually part of a plant's natural defenses that keeps it from being decomposed. But it is also a major roadblock for researchers eager to find ways to extract a plant's sugars to develop ethanol, advanced biofuels, and other chemicals. Researchers are seeking different methods to deconstruct abundant, renewable lignocellulosic biomass to access its sugars as essential intermediates for conversion to biofuels.

To unlock these sugars, scientists at NREL are using innovative computational-based studies to explore solutions to this problem. The NREL researchers are improving our understanding of the scientific basis for plant recalcitrance, so that they can develop sustainable feedstocks that are easier to deconstruct. They are also working to learn more about cellulase and hemicellulase enzymes that can quickly and inexpensively produce sugars from lignocellulosic biomass such as corn cobs and stalks, switch grass, poplar trees, and woody residues.

Pursuing an *in silico* Approach

For more than 30 years, NREL researchers have made significant experimental advances in understanding the intricacies of polymers found in plant cell walls, as well as the difficulties involved in breaking down the polymers to fermentable sugars. But while experimental studies are critical, this research approach can face daunting challenges in trying to fully understand the complexity of polymers within plants, across spatial scales spanning the atomic to macro.

To accelerate this understanding, NREL scientists increasingly use computational (or "in silico") studies to complement their experimental work. Computational results can provide insights that are inaccessible through experiment, while also identifying the next set of experiments to pursue to confirm or reject given hypotheses. The in silico approach, which includes modeling, simulation, and visualization, targets:

- Understanding basic phenomena—for example, what is the detailed nature of cell walls, microfibrils, cellulose, and hemicellulose? How are cell wall structure, chemistry, and enzyme activity interrelated?
- Using the deepened understanding to develop improved processes to deconstruct cell wall polymers to sugars—for example, significantly boosting the amount of biomass substrate that is converted to sugars, measured against how long it takes and how much enzyme is required to make the conversion happen. Finding enzymes that are more effective, thermally

stable, and lower in cost will facilitate industrial production of biofuels from lignocellulosic biomass.

Starting with Cellulose—One Tough Material

Cellulose is a carbohydrate polymer—long chains of linked glucose molecules called cellodextrin, with these long chains combining to form crystalline bundles. Researchers have characterized several different crystallographic forms of cellulose, including natural forms found in plant cell walls, and various crystalline forms created by treating natural cellulose with chemicals such as ammonia or ionic liquids.

Recently, NREL scientists have used the RedMesa supercomputer at Sandia National Laboratories to determine the thermodynamic work required to remove a single cellodextrin chain from four different forms, or crystalline polymorphs, of cellulose. The computational analysis revealed that it takes about an equal amount of thermodynamic work to remove a cellodextrin chain from natural plant celluloses (polymorphs Iα and Iβ), whereas removing a cellodextrin chain from cellulose II and III—two polymorphs that come from chemically pretreated natural cellulose—is considerably easier. This implies that celluloses II and III will be less recalcitrant, or resistant, to enzyme deconstruction than natural plant cellulose. These results provide critical understanding that can help guide future development of biomass pretreatment processes and potentially enhanced biological catalysts and genetically engineered plants, which may significantly reduce the cost of producing lignocellulosic biofuels.

In other studies, NREL scientists modeled cellulose microfibrils to learn how temperature affects the structure of plant cell walls at the nanoscale. Individual microfibrils are cellulose chains twisted together into ropelike structures that can be thousands of nanometers long, but are only 3.5 nanometers thick. Heating, which is part of the biomass pretreatment process, causes many changes in the cell wall; but these are difficult to study experimentally and therefore have not been well understood at the molecular level. Through molecular simulations, however, researchers learned that heating is predicted to cause the cellulose microfibrils to straighten. As a result, the microfibrils' "twist" is compressed into short regions with reduced crystallinity that may be easier to break down. The simulations also provide an explanation for experimental observations that heat-treated cellulose deconstructs significantly faster at the beginning of hydrolysis (the chemical reaction that breaks the bonds in the cellodextrin chain) than at the end. NREL scientists hypothesize that the highly twisted regions are more susceptible to hydrolysis and break down first, while the straighter regions remain recalcitrant.

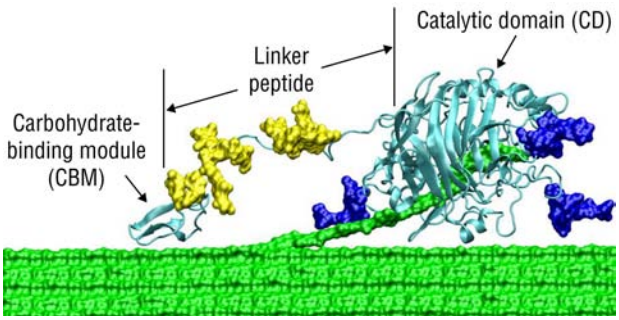
Getting to Sugars—Deconstruction by Enzymes

In nature, fungi and bacteria use cocktails of enzymes to digest biomass. Although there are numerous individual enzymes involved, the enzymes that deconstruct cellulose can be classified as one of three basic types.

The first type of enzyme is an endoglucanase. Endoglucanases attack single cellodextrin chains within the interwoven network of crystalline cellulose fibers. Endoglucanases cut the cellodextrin chains in the middle, creating two new chain ends in the process.

The second type starts working where the first leaves off. This enzyme, which is called an exoglucanase, attaches itself to one of the new loose ends and pulls the cellulose chain out of the crystal structure. The end of the chain threads into a tunnel or notch in the enzyme, and it is cut by the exoglucanase into cellobiose, a disaccharide containing two linked glucose molecules similar to table sugar.

The third type of enzyme, a beta-glucosidase, catalyzes the hydrolysis reaction between water and cellobiose units, and cuts them into their glucose molecules. This glucose can then be fermented into ethanol, butanol, hydrocarbons, or other biofuels.



The cellobiohydrolase enzyme from T. reesei consists of three sub-domains: (left) a carbohydrate-binding molecule (CBM); (middle) a linker peptide with attached polysaccharides (yellow); and (right) a catalytic domain (CD) with attached polysaccharides (blue). A single cellulose chain from the cellulose microfibril (green) is hypothesized to thread into a tunnel in the CD; the chain is cleaved and the two-sugar product, cellobiose, is expelled from the right end of the tunnel.

Growing NREL's Computational Arsenal

In pursuing their computational work, NREL scientists encounter modeling issues across multiple scales. Some research problems require analysis at the atomic level; others at the scale of macromolecular interactions; and others at a coarser-grained scale of an entire system. In terms of spatial dimensions, the scale of these models may span from less than a nanometer (10^{-9} m) to micrometers (10^{-6} m).

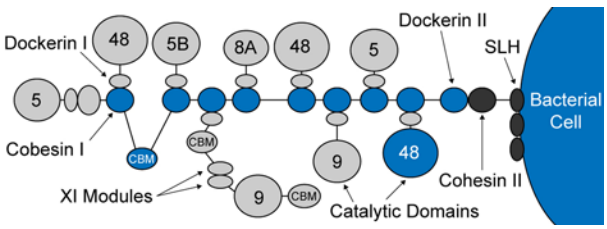
Time scale is also an issue. When extremely large numbers of calculations are necessary, the sheer magnitude of processing cycles constrains the simulation time. Depending on the problem being addressed and techniques used, the time scale may range from femtoseconds (10^{-15} s) to milliseconds (10^{-3} s).

Considering these spatial and time scales, NREL's ongoing goal is to develop better techniques that are coded into better applications that run on better computing systems. Better techniques imply more accurate, powerful means to describe underlying physical and chemical processes. As an example, using improved force-field parameters may result in a more accurate description of cellulose structure.

To improve the software they use, researchers have to find ways to translate their improved techniques to computer code that is also better designed, more efficient, and more flexible analytically. To achieve this, NREL is leading a project, funded by U.S. Department of Energy (DOE) Biological and Environmental Research and DOE Advanced Scientific Computing Research (SciDAC), to build better molecular dynamics codes.

Finally, high-performance computing (HPC) provides the all-important increase in computational power that researchers require. NREL is constructing an Energy System Integration Facility that will house a new HPC data center. When operational in 2012, the supercomputer will have a processing speed of one-half petaFLOPS—0.5 quadrillion or 1015 floating-point operations per second—with plans to expand to one petaFLOPS. This world-class HPC capability will permit more sophisticated models to be developed and run.

The typical exoglucanase has three "sub-domains," shown in the following figure. To reduce the number of atoms involved in the simulations and thus reduce the computational resources required, many functions of the enzyme can be computationally modeled by focusing separately on each domain. For example, NREL researchers have examined the movement of the carbohydrate-binding molecule (CBM) on the surface of cellulose microfibrils by combining computational analysis with experimentally determined three-dimensional structures. A key result of this research is the discovery of attractive attachment locations, or "energy wells," for movement of CBMs on cellulose surfaces that are spaced one nanometer apart. These energy wells are a natural fit for the CBM, and their spacing equals the dimension of two glucose units in the cellulose crystal, which is the distance required for the intact enzyme to move to produce the cellobiose product.



Cartoon of cellulosome from C. thermocellum, where scaffoldin subunit (dark blue) contains nine cohesins and a carbohydrate-binding module (CBM). Cellulolytic enzymes (gray) bind to cohesin partners with their dockerins. Another set of dockerin/cohesin interactions connect the scaffoldin to the cell wall via a protein (SLH).

Researchers studying the catalytic domain (CD) are also using computational analysis. Their technique estimates the energy barriers between elementary steps in the enzyme-catalyzed reaction, and identifies where the most significant energy barriers exist. Specifically, their free-energy calculations predict the energies required to thread the cellodextrin chain into the tunnel, hydrolyze the chain into cellobiose units, expel the cellobiose product, and advance the cellodextrin chain into another cellobiose unit to prepare for another hydrolysis step. The researchers have gained further insights about what occurs at a

molecular level using techniques such as rare-event simulation to study threading, quantum mechanical/molecular mechanics to study the hydrolysis mechanism, and steered molecular dynamics to study cellobiose product expulsion. In the study of cellobiose expulsion, computer simulations of the expulsion provided data that helped researchers suggest mutations in the exoglucanase catalytic domain to enhance the product expulsion step. These suggestions are presently being incorporated into engineered enzymes to test the predictions.

Unlike enzymes produced by the fungus T. reesei, those found in the bacterium Clostridium thermocellum form a cellulosome, which is a very large multi-enzyme complex. The cellulosome is like a "multi-member demolition crew" dedicated to the job of attaching to a plant cell wall and working synergistically to dismantle the cell wall's polymers into sugars.

Structurally, cellulosomes are made up of a scaffoldin, which is a long flexible protein that has specific binding sites called "cohesin domains," and multiple enzymes that have dockerin modules that bind to the cohesins. The cellulosome self-assembles because the dockerin modules on the enzymes recognize complementary cohesin sites on the scaffoldin.

Researchers are not yet sure exactly how this particularly effective nanomachine works. They do know that Clostridium thermocellum secretes enzymes and scaffoldins that self-assemble outside the organism. Because NREL's researchers want to better understand this molecular self-assembly process—as well as the computational resources needed to perform an atomistic simulation—they created a "coarse-grained" computational model containing only features that significantly contribute to the properties they want to simulate. The researchers assumed that the subunits' molecular weight, flexibility, and affinity for each other would have the greatest influence on the self-assembly.

The scientists ran thousands of models that used different enzyme concentrations and ratios to simulate representative environments that the scaffoldin and secreted enzymes encounter near the bacterium cell wall. They compared their results directly with the results of experimental studies of binding affinity. The modeling yielded a significant counterintuitive result: larger enzyme subunits are assembled more quickly than small subunits onto the scaffoldins. The enhanced binding of larger enzymes was shown to result from their slower diffusion and greater flexibility. Consequently, they are more likely to entangle with and bind to the scaffoldin. In contrast, the smaller enzymes move more rapidly and are less likely to bind to the scaffoldin.

Researchers will apply what they learned about binding affinities to control the ratios and perhaps the locations of enzymes on the scaffoldin that have synergistic functions. They will use what they understand about the binding affinity to engineer the enzymes' desired catalytic function. Their ultimate goal is to make artificial, or engineered, cellulosomes that are designed to work more effectively on specific pretreated biomass feedstocks. To this end, NREL has constructed a minicellulosome—a scaled down but fully functional version of larger natural multi-enzyme complexes—to advance the concept of cellulosome designs and create enzymes that more effectively catalyze cell wall deconstruction.

Shedding Light on the Science to Spur the Technology

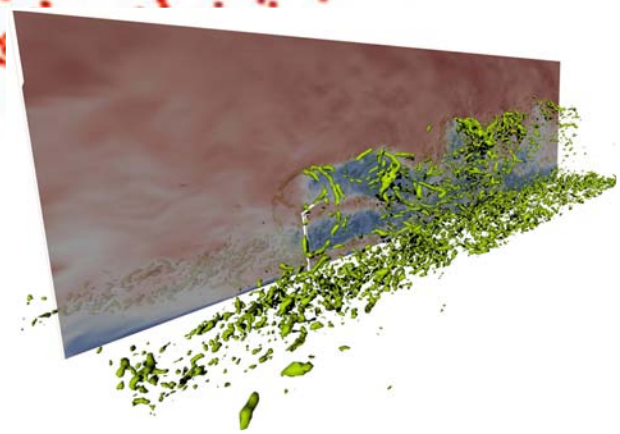
NREL researchers, working with academic and industrial partners, have shown that combining experimental studies with computational modeling produces understanding that they can successfully apply to large, complex biological systems. By attacking industry-relevant problems with exactly this sort of rational, integrated approach, they expect their work to lead to engineered and optimized enzymes able to deconstruct specific types of biomass. To achieve this goal, researchers will have to:

- Better understand how cellulases and other enzymes work that degrade cell wall polymers
- Predict the best place to make changes within the enzymes to improve them
- Actually make the specific changes
- And, finally, test the products or processes to confirm the beneficial outcome.

As NREL sheds light on the intricacies of the science underlying the conversion of renewable biomass resources to biofuels and chemicals, the laboratory is helping lay the solid foundation for developing the next-generation technologies that will enable the industry to produce large volumes of biofuels cost effectively.

—Don Gwinner

Supercomputing Drives Innovation



Large-eddy simulation (LES) of a neutrally stable atmospheric boundary layer with the wind turbine blade aerodynamics modeled using actuator lines. A vertical cross-section shows streamwise velocity magnitude (red represents high velocities, whereas blue represents low velocities); notice the development of the low velocity wake behind the turbine. The green isosurface is the q-criterion (second invariant of the velocity gradient), showing the vortical structures trailing from the blade.

Researchers are finding new ways of tackling our nation's energy challenges.

Using NREL's computing power, researchers are identifying optimal components, processes, and systems that are leading to new ways of tackling our nation's energy challenges—avenues that simply are not always viable through trial-and-error or traditional experimentation alone.

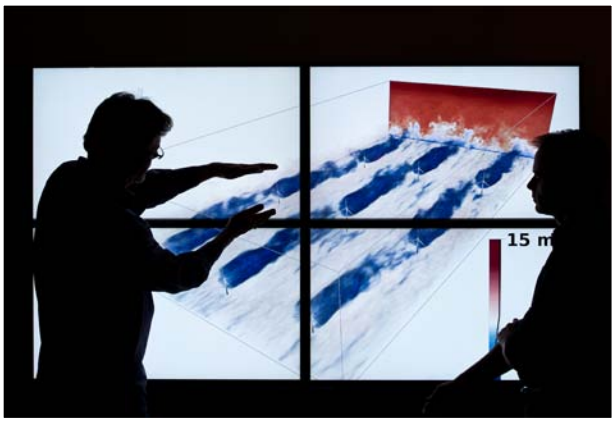
NREL's brawny computers help researchers do the heavy lifting across a range of fields, from biofuels to photovoltaics (PV). These computers are also being used to advance energy efficiency in buildings. RedMesa, currently NREL's most powerful high performance computing (HPC) system, has a peak capability of about 180 teraFLOPS, performing 180 trillion "FLOPS," or floating point operations per second (see page 9 sidebar). This computer, which is co-located with the larger RedSky HPC system at the U.S. Department of Energy's Sandia National Laboratories, has proved so popular with researchers that NREL scientists have kept the system running at capacity—day and night—for the past year.

For example, during a recent nine-month period, scientists from NREL and its collaborators used 7.5 million computational hours on RedMesa to evaluate more than 30,000 candidates in their pursuit of promising organic photovoltaic (OPV) cells. If these analyses had been done experimentally in a laboratory, they would have taken around 7,000 person-years to create and study that many different materials. So far, this sort of computational analysis has identified more than 300 highly promising materials, 10 of which are in the synthesis pipeline, ready to undergo further evaluation.

As demonstrated by this time savings, NREL is relying on HPC systems to drive technology innovation that is vital to the lab's research and development. The HPC system capabilities now allow scientists and engineers to thoroughly explore a dizzying array of possible designs, configurations, and alternatives in virtual experiments. This potent tool is also being used to explore new horizons in biomass, solar, and wind energy technologies.

High-Performance Computing Accelerates Biofuels Research

To ensure that cellulosic ethanol and advanced fuels are produced at costs competitive with fossil fuels,



NREL's Steve Hammond, Director of Computational Science Center and Kenny Gruchalla, Senior Scientist, discuss a 3D model of wind plant aerodynamics, showing low velocity wakes and impact on downstream turbines.

researchers rely on NREL's HPC capability to analyze the complex chemistries and dynamics involved in both thermochemical and biochemical pathways for more efficient biofuels production.

For instance, NREL scientists are using HPC to understand how naturally occurring enzymes from fungi and bacteria break down plants in nature, with the overall aim to then use this knowledge to design enhanced enzymes that will reduce production costs for biofuels. Much about the behavior of these enzymes is unknown, and the plant walls themselves are quite complicated and poorly understood. Over the past two decades, however, research groups have gained crucial understanding about the structures of important enzymes found in nature. Leveraging this knowledge, in recent years, NREL scientists have used supercomputers to simulate 3D models of the primary enzymes and cellulosic materials involved in biofuel production. This work has led to a surge of computational experiments that have identified previously unknown functions in these enzymes, and has suggested further experimental work to tackle this challenging problem.

By employing RedMesa and other supercomputers, scientists can model the complex microfibril structure of cellulose from plants and create visualizations that help explain how enzymes break down feedstock such as corn stover and poplar trees for renewable fuels. For the enzymes that break down plant cellulose, NREL researchers have probed single enzymes from the industrially important fungus, Trichoderma reesei, and enzymes from the bacterium Clostridium thermocellum. These two organisms are very effective biomass degraders in nature, but have significantly different means of breaking cellulose down into basic sugars. Understanding the suite of enzymes from both of these organisms can provide key insights for biologists to produce enhanced enzyme systems for industrial biofuels processes. Overall, this computational approach has helped researchers better understand basic science of both the plant cell wall structure and chemistry, as well as helped them design improved processes involving enzymes to break down the cell wall. See the *Continuum* article on biomass in this edition (page 15).

These sorts of inquiries support both the Obama administration's goal of a timely and efficient transformation of the nation's energy system and the U.S. Department of Energy's target of securing American leadership in clean energy technologies. The administration has proposed an 18% cut in daily petroleum consumption in less than a decade, which translates to a reduction of 3.5 million barrels per day, from a 19-million-barrel baseline, by 2020. To replace some of that fossil fuel volume, DOE has set a goal of having 60 million gallons of biofuels in the nation's supply by 2030.

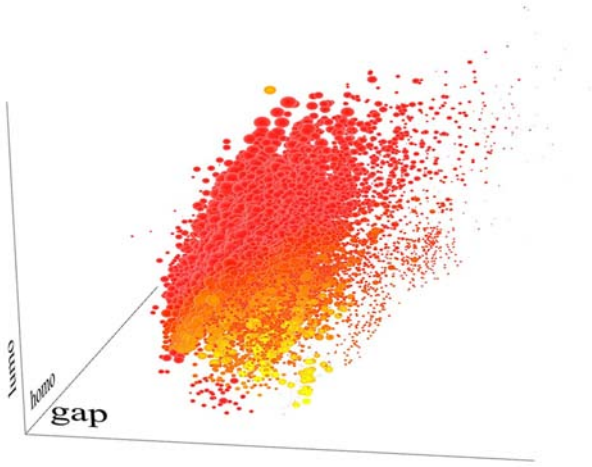
Fine-Tuning Solar Materials with HPC

Biofuels research is not the only program making use of HPC capability. Photovoltaic researchers also employ HPC to help design novel materials that have the exact properties required to dramatically improve solar cell performance. The researchers are also using HPC to identify unique materials that have radically improved thermal energy storage and stability characteristics in order to create low-cost, highly efficient concentrated solar power systems.

As mentioned previously, OPV cells show great promise as lightweight and flexible devices to convert sunlight to electricity. Currently, the best OPV devices have power conversion efficiencies approaching 10%, and are more than twice as efficient as they were just three years ago. These dramatic gains have been possible because researchers have been able to chemically tune material used in the light-absorbing active layer so that it can better absorb sunlight and generate more power generation for every photon it absorbs. This kind of continued improvement in OPV performance depends on the discovery of novel active layer materials that can convert photons into power more efficiently.

The main constraint is that new materials may require several months to synthesize, which means that researchers have created and tested only a few

hundred out of tens of thousands of plausible candidates. To circumvent this bottleneck, NREL computational scientists, along with organic chemists and material scientists, developed a high-throughput computational screening method to test active-layer materials.



A three-dimensional scatter plot showing computed electronic properties of tens of thousands of potential OPV materials that were auto-generated according to combinatorial rules. The points are sized by the overlap of their absorption spectrum with the solar spectrum, and colored according to "fitness" which is proportional to the predicted OPV device efficiency (yellow is more efficient, red less efficient).

> *"The continued rapid advances in supercomputing capability are now enabling scientists to conduct detailed simulations of large wind farms or explore the fundamental properties of entire classes of materials—problems that were intractable just a few years ago."*
>
> — Steve Hammond, director of NREL's Computational Sciences Center

Typically, researchers screen these sorts of candidate materials in a four-step process that starts when new materials are generated combinatorially, in which computer scientists analyze large sets of data. Researchers leverage a large library of chemical building blocks and then perform high-level electronic structure calculations on them. The results are processed and automatically imported into a searchable database, creating an OPV material database similar to that of the human genome. The materials with the desirable electronic properties are then shared with chemists to synthesize and characterize.

Supercomputers Provide a Picture for Improved Wind Farms

NREL scientists and engineers develop innovative software tools to simulate the behavior of both individual wind turbines and multi-turbine configurations in complex environments, such as high winds, extreme turbulence, and even hurricanes. This kind of advanced software models the effects of turbulent inflow, including unsteady aerodynamic forces, and the inflow's effect on structural dynamics and drive-train response. Even before offshore wind turbines exist in US waters, these sorts of models can test hydrodynamic loading, helping to ensure that the best possible designs are deployed.

To improve these models, their results must be compared with actual observations. NREL has a long history in collecting data that describes the efficiency and reliability of turbines. In early 2011, an interagency group comprised of NREL, the University of Colorado at Boulder, the National Oceanic and Atmospheric Administration, and DOE's Lawrence Livermore National Laboratory, deployed high-resolution atmospheric instrumentation at NREL's National Wind Technology Center to study the atmospheric flow fields surrounding large wind turbines. The team collected meteorological data in order to validate turbine wake models in a range of atmospheric stability conditions. Understanding and predicting wind plant aerodynamics and the impact of turbulence from upwind turbines on downwind turbines is vital when optimizing wind plant turbine layouts as well as designing turbines with longer lifespans. The interagency study's data will provide valuable insights into the operation and optimization of these large wind turbines.

This type of knowledge could reduce the cost of electricity generated from wind energy, as these insights enhance wind farm efficiency and help extend the life of wind turbines. This research could also help offshore studies, and support the path to DOE's benchmark to cut the levelized cost of wind energy.

NREL's HPC Future Is Taking Shape

NREL has already leveraged its current HPC capabilities to help meet critical goals in biofuels, wind energy, and PV for DOE and its Office of Energy Efficiency and Renewable Energy. However, just as the capabilities of computers continue to expand to meet demands, so does

NREL's HPC systems capacity, enabling integration across a wide range of applications.

- Vehicles: NREL's HPC capabilities will be able to model system design and material thermal properties for power electronics, advanced batteries, and renewable fuels combustion properties
- Buildings: NREL will be able to determine the optimal cost and energy performance solution sets for energy efficient building retrofits, and for new ultra-efficient and net-zero-energy buildings
- Hydrogen: the HPC will simulate the thermal and structural properties of fuel cells for marked improvements in fuel cell performance, durability, and thermal management
- SmartGrid: the capacity to model and simulate grids will help the power industry better understand the evolution to a cleaner, reliable, efficient, and secure grid that includes high penetration renewables.

NREL researchers' ongoing use of the RedMesa HPC system has demonstrated how essential this sort of computer analysis is to their work. When the lab's Energy System Integration Facility (ESIF) is completed in late 2012, NREL plans to acquire a new HPC system with more than double RedMesa's computational capability.

As NREL continues its leadership in advancing renewable energy and energy efficiency technologies—working to help attain administration and DOE energy goals—it continues to find ways to leverage growing HPC capacity to support advances in areas including energy efficient buildings, photovoltaics, wind energy, biofuels, and other renewable energy and energy efficiency technologies. While the petascale era dawns at NREL with the planned petaFLOPS supercomputer, NREL computational scientists and researchers remain committed to staying in the forefront of renewable energy and energy efficiency research while continuing to embrace the laboratory's mission of sustainability.

—Ernie Tucker

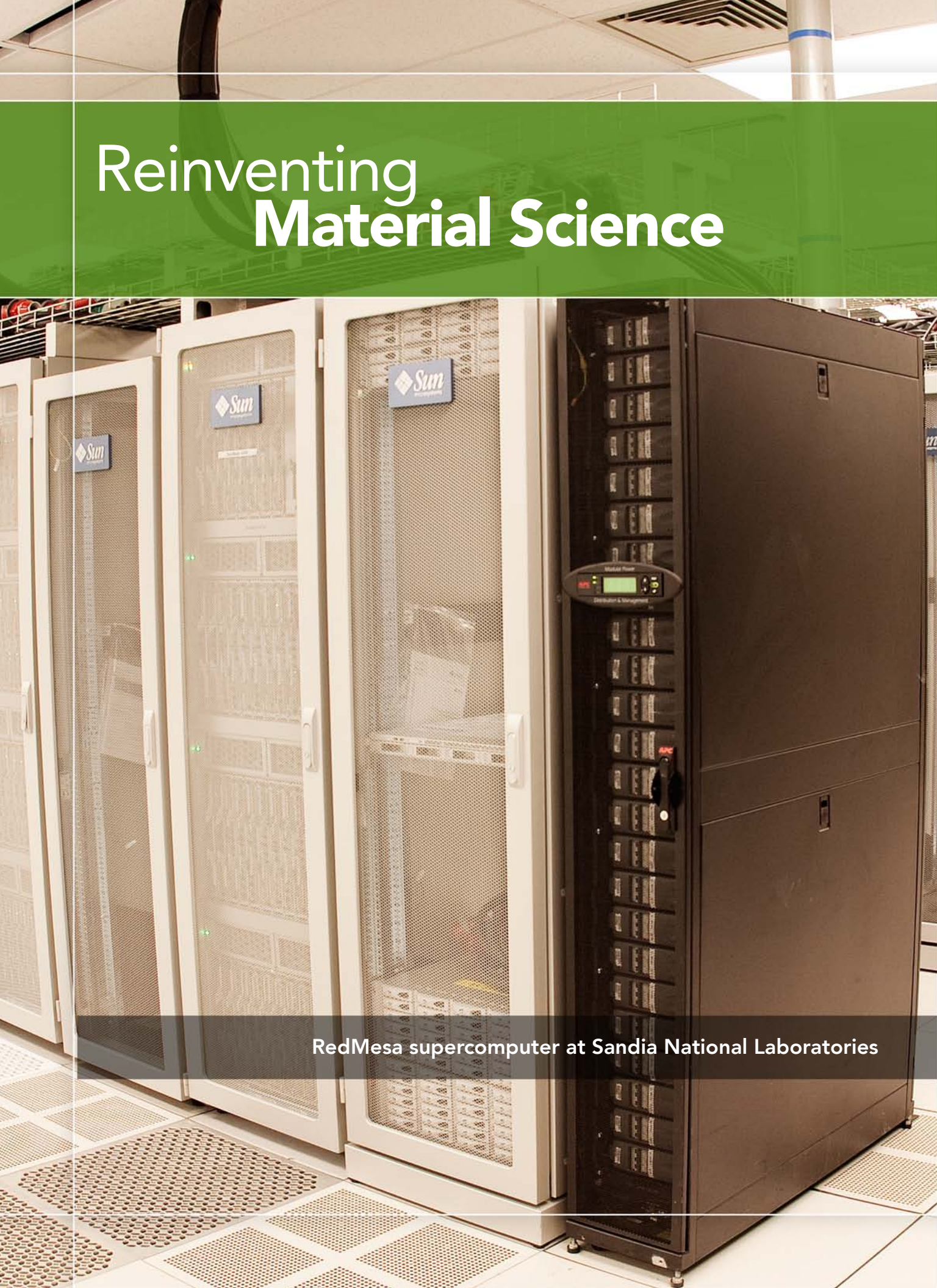
NREL's New Green Data Center Will Be a Green Giant

Even though its new HPC system is still under development, NREL is preparing for its expected petaFLOPS level. To understand how powerful this sort of system is, imagine if each of the 7 billion people on Earth had hand calculators and worked together for 24 hours a day, 365 days a year on a calculation. Under that scenario, it would take more than 16 years to do what a petascale supercomputer can do in one day. These HPC systems, the world's most powerful, can perform 1015 operations per second.

As it draws on supercomputer capabilities, NREL remains true to the laboratory's mission of walking the talk in support of sustainability. With the expected completion of the new ESIF facility, the immense computing tool being built to function without using the immense quantities of energy typically associated with cooling and facility infrastructure of a typical HPC system. The new ESIF's ultra-energy-efficient HPC data center is being designed to be the world's most energy efficient data center.

Because of its efficiency, annual operating costs for data center power and cooling will be about half of the operating costs of a typical data center. Additionally, waste heat from the high performance computing equipment will be captured and used as the primary heating source for office and laboratory space, further reducing energy consumption and operational costs for the ESIF.

Reinventing **Material Science**



RedMesa supercomputer at Sandia National Laboratories

It's not often that scientists set out to reinvent an entire field of study, but it's happening now.

It's not often that scientists set out to reinvent an entire field of study, but that is exactly what the Center for Inverse Design is pursuing in the field of material science. The vision of the center is to revolutionize the discovery of functional materials by developing an "inverse design" approach, powered by theory that guides experiment.

The Center for Inverse Design was established as an Energy Frontier Research Center, funded by the U.S. Department of Energy's Office of Basic Energy Sciences. The National Renewable Energy Laboratory (NREL) is the lead organization in partnership with Michael Toney of the Stanford Linear Accelerator Center; professors Arthur Freeman, Thomas Mason, and Kenneth Poeppelmeier of Northwestern University; professors Douglas Keszler and John Wager of Oregon State University; and Alex Zunger, formerly of NREL and now at the University of Colorado at Boulder.

Historically, the development of new materials for technology has been largely based on trial-and-error search or even accidental discovery. The Center for Inverse Design is founded on the key principle that modern theory, combined with high-throughput and targeted experimentation, can directly address the challenge of innovating novel materials and nanostructures by design. This principle takes the conventional paradigm and reverses it—given the desired property of a material, find the structure of the material. Theory can then guide experiment, rather than simply describe its results.

This Holy Grail of materials science is becoming reality due to the availability of ultra-high-speed computing, the creation of high-throughput experimental tools and iterative techniques, and the development by Zunger and his colleagues of "inverse band structure"—a method of deriving crystal structures based on predetermined electronic and optical properties—as well as other theoretical approaches. This powerful combination had not existed before.

NREL Research Fellow David Ginley (center) and NREL post-doc Paul Ndione operate NREL's new pulsed-laser deposition system, which allows them to deposit multiple gradated films on top of one another. This process can create thousands of different compounds on a single 2-inch-by-2-inch substrate.

"The Center for Inverse Design represents a new way of approaching science," says William Tumas, the center's director. "Our approach to inverse design can be pivotal by coupling theory and experiment. This can significantly accelerate the rate of basic science discovery."

The Key for High-Throughput Computation: Supercomputers and Algorithms

"Historically, if you told other material scientists that you were going to do inverse design, they would look at you and laugh," says NREL Research Fellow David Ginley, the center's chief scientist for experiment. "That's literally true, because there wasn't enough computational power—doing one material was hard, doing 100,000 or a million was just ridiculous. You couldn't think about doing that much calculation in a reasonable way."

Supercomputers have allowed the center to succeed in its new approach, but so have a number of algorithms that allow the researchers to perform those calculations more efficiently. For the initial focus of the center on semiconductor materials used in solar cells, many of those algorithms were developed at NREL, drawing on its 30-year history of developing solar cells and learning how solar cells and other semiconductor-based devices function. By combining supercomputers and efficient algorithms, the center has opened the door to new material science.

"In the old days, if you wanted somebody to calculate the properties of a cluster of atoms, they'd

come back and say, 'We can do ten atoms,'" says Ginley. "Well, ten atoms do not a material make, and so calculating bulk materials properties was tough. But by going to new ways of doing the calculations, we now can do hundreds to thousands of atoms, and those are much more representative of a real material."

Stephan Lany leads the NREL theory component of the center. He and his colleagues have developed and applied methods to predict material properties based on first principles, using calculations of electronic structures. They have implemented approaches to predict, with a high degree of reliability, experimentally relevant properties of semiconductor materials, such as the structure, doping, and electron-carrier concentrations, as well as bandgaps or absorption spectra. This predictive capability is essential to design materials with target properties and functionalities.

"By coupling these tools to today's high-performance computing resources, we can quickly evaluate a large number of potential materials in a way that we've never done before," says Lany. "This enables inverse design to work and will lead to the realization of new and optimized functional materials through an iterative approach that draws successively on theory, experimental synthesis, and characterization."

High-Throughput Synthesis: Like Spraying Paint

To make a broad spectrum of potential materials, the Center for Inverse Design uses combinatorial methods to build "composition-spread libraries" of materials. To do this, researchers create 2 x 2" squares that gradually change in composition from top to bottom and from side to side. As a result, each point on the square represents a unique material composition. That may sound difficult, but in practice, it's not.

"It's really easy," says Ginley. "It's like we have a yellow, a blue, and a red spray-paint can, and we spray overlapping color circles onto the substrate. Where the circles overlap, we get every combination."

In reality, instead of using spray paint, a process called sputtering deposits the materials on the substrate. In sputtering, energetic particles free the atoms from a piece of source material, and then these freed atoms pass through a nozzle—a "sputter gun"—that sends them hurling onto the substrate. During sputtering, "basically, each sputter gun acts like a spray source for a particular atom or compound," says Ginley, "and when you co-deposit these materials, you get intimate mixing, and so you get everything in the range of materials that you're looking for."

NREL is using the RedMesa supercomputer at Sandia National Laboratories to perform its complex computations, including calculations of the physical properties of thousands of potential solar-cell materials. NREL will have its own supercomputer when the Energy Systems Integration Facility, now under construction, is completed late this year.

Researchers can also deposit the materials using a process called pulsed-laser deposition, which uses pulses of laser light to vaporize the surface of a source material. Some materials can even be dissolved in solvents or suspended in solutions and deposited using ink-jet printers.

To explore an even wider range of materials, researchers can also change the conditions under which the film is deposited, perhaps by changing the deposition temperature across the width of the square, or by varying the partial pressure of oxygen in the deposition chamber across the height of the square.

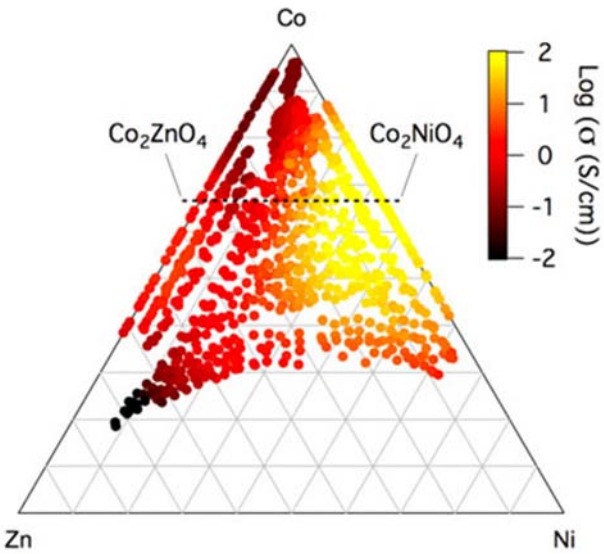
High-Throughput Analysis and the Data Crunch

Once researchers have created the 2 x 2"-square compositional library, there are several analytical techniques they can use to measure its properties. Because each point on the square represents a different material composition, taking an array of measurements across its width and breadth yields a wealth of data.

For example, researchers might measure the library's electrical conductivity, light absorption, light reflection, and its work function, which is the minimum energy needed to free an electron from its surface. Considering that each point in the library could have at least a couple process variables and four or five physical property measurements associated with it, that's a lot of variables to consider.

If you wanted to create a plot of how all those variables related to each other, the plot would easily have seven dimensions to it, or maybe more. This is why finding the sweet spot for material with the desired properties turns out to be one of the center's greatest challenges.

"It's like doing this huge array of material science in one fell swoop," says Ginley. "Of course, you generate terabits of data, and the real question is: how do you take these huge data files and mine them appropriately to get the real information out? And that's still an evolving area.



An example of high-throughput material science is shown in this ternary graph of electrical conductivity (in Siemens per centimeter) for one thousand oxides containing zinc, nickel, and cobalt, all of which were deposited on a single 2-inch-by-2-inch substrate as overlapping, gradated films containing each of the metallic elements. Co_2NiO_4 was found to be the most conducting sample.

"People are okay thinking about one, two, or three dimensions, but when you're up to 10, not a chance! So how you mine the data and how you present it in a way that you can make logical conclusions from it is non-trivial."

Zeroing in on an ideal material is also an iterative process, so there may be several material libraries loaded with data for each investigation. For instance, if an initial material library examines an oxide with a cobalt content ranging from zero to 100%, and finds a material sweet spot around 25% cobalt, a second material library might examine a cobalt content running from 20% to 30%. A third might zero in on a tighter range, such as 22%–23%. Each step is like zooming in with a microscope on a particular area of interest.

Once the center's researchers find an apparently "ideal" composition, they revert to more traditional material science approaches: synthesizing that ideal composition, characterizing the material, and applying theoretical analysis to fine-tune its material properties.

Proving the Model of Inverse Design

The center's work on spinels has already proved that its approach can work: by first using theory to derive a set of "design rules" for p-type spinels, researchers applied those rules to achieve a 10,000-fold increase in conductivity in one potential material.

"The approach and tools that we've developed through the extensive capabilities within the Center for Inverse Design are starting to show the value of the inverse design approach for materials discovery," says Tumas.

Despite those challenges, the center has already accomplished far more than would have been possible just a few short years ago.

"We can cover in a week what used to take a researcher's entire post-doctoral career, literally," says Ginley. "Being able to do material discovery as fast as the theorists can do the theory creates the ability to really carry out inverse design."

And although the center is currently focused on improving solar cell materials, its work could potentially establish inverse design as a new, proven approach to material science in general—an approach that could be applied to all types of materials challenges.

"We are focusing on synthesizing predicted materials for solar energy conversion and also looking into other desired properties of materials," said Tumas. "We still have a ways to go to make inverse design truly a reality that will be adopted by the materials science community. Larry Kazmerski, our program integrator, is leading our efforts to reach out to that community. So the solar cell materials—while important and significant in their own right—are also the means to an end of actually validating that inverse design works."

—Kevin Eber

Partnering to Solve Solar Cell Material Challenges

The Stanford Linear Accelerator Center (SLAC), one of the partners in the Center for Inverse Design, is providing the center with access to its Stanford Synchrotron Radiation Lightsource, which produces extremely bright X-rays that can be used to study materials on the atomic scale.

"SLAC has capabilities for measuring atomic positions and which elements are in particular positions that we can't do elsewhere—that you basically can't do anywhere that doesn't have a big synchrotron-based X-ray source," says John Perkins, a senior NREL researcher for the center. "The interactions with SLAC are critical to closing the loop, allowing us to determine if the atomic structures are causing the resultant material properties in the way that we expect them to."

One example is the center's work on spinels, a type of oxide with the form A_2BO_4, in which A and B are positively charged atoms. Because spinels can be transparent and can conduct electricity, they are used to form the top layers of solar cells. This top layer conducts electricity out of the cell while allowing light to pass through to the heart of the solar cell. The center is currently investigating "p-type" spinels, which are better at conducting the positively charged "holes" left behind by vacant electrons, rather than conducting the electrons themselves. This capability allows the spinels to serve as a positive terminal. In contrast, "n-type" materials conduct negatively charged electrons better than holes and serve better as negative terminals.

"If we take a prototypical spinel material, such as Co_2ZnO_4, our calculations predict that if the zinc ends up on a cobalt site in the crystal lattice, that's good—that creates free holes that lead to p-type conductivity. However, if the cobalt ends up on a zinc site, that's neutral and it doesn't make any difference in the material," says Perkins. "And it's predicted theoretically that the number of cobalt atoms on zinc sites will be far, far greater than the number of zinc atoms on cobalt sites, but because the cobalt atoms on zinc will be neutral, the material will still turn out to be a p-type conductor.

The NREL-led Center for Inverse Design is employing the Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC to study solar cell materials on the atomic scale. The SSRL accelerates electrons to near the speed of light in an oval path defined by a ring of electromagnets, called a synchrotron. The electrons emit extremely bright X-rays as they follow this path, and this radiation is used to study matter.

"We can determine that it's a p-type conductor at NREL, but we can't determine how many cobalt atoms are on zinc sites and how many zinc atoms are on the cobalt sites, so we can't determine whether or not the mechanism that's been predicted theoretically is actually the mechanism at play that's causing this to happen. That's why we have to go out to SLAC. That's generally true for the materials being worked on at the center: basically, the resultant material properties will depend in detail on which atoms are in which sites, and that information is the information we get out of SLAC."

According to NREL Research Fellow David Ginley, the collaboration has been even more successful than anticipated.

"It has been so beneficial that it has become addictive," says Ginley. "Originally we had a couple people going out to SLAC; now we have people going out all the time. They can examine atomic structure and site occupancy, they can examine electronic properties, and they can do it all at a level of resolution that we just can't touch at NREL.

"This is really a true collaboration. We're not just going out there and running samples, we're intimately working with the people out there, and that work is accelerating our understanding and our rate of progress."

Rewiring Algae's Catalytic Circuits

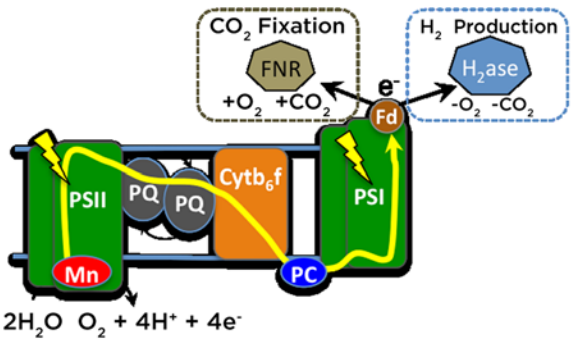
Opening a promising avenue to increased biohydrogen production.

In nature, photosynthesis uses the energy in sunlight to split water into carbon dioxide and hydrogen. A typical plant cell relies on a series of electron carriers, which create a photosynthetic circuit that allows plants to capture the carbon dioxide they need, and then convert it into the biomass that fuels cell growth. At the same time, plants produce hydrogen, a molecule that can be used in a variety of renewable and sustainable fuel technologies, but that is also expensive to produce in large quantities and currently involves non-renewable natural gas reformation.

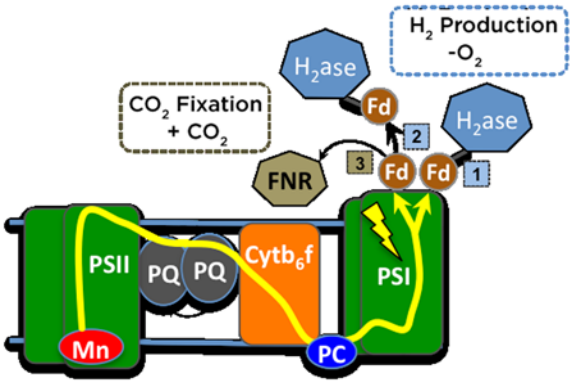
A photosynthetic organism such as green algae tends to use solar energy to generate either fixed carbon or hydrogen—while this is fine for growth, it is not particularly efficient for making greater quantities of hydrogen. Facing this challenge, NREL researchers wondered if they could find ways to boost the hydrogen-making capacity of photosynthesis. They posed a key question: What controls the partitioning of electrons between these two competing metabolic pathways?

A team from NREL, along with colleagues from the Massachusetts Institute of Technology and Tel Aviv University, set out to answer this question. They hypothesized that they could engineer the process by "rewiring" algae's catalytic circuits, or pathways. To do so, they would replace the normal hydrogen-producing enzyme, hydrogenase (H_2ase), with a ferredoxin and hydrogenase fusion protein. They speculated that inserting this kind of a fusion protein into this reaction path could divert more electrons into hydrogen production and push the algae into making more hydrogen and fixing less carbon dioxide. If successful, this engineered photosynthetic circuit could potentially increase efficiencies and thus bring down the price of hydrogen. In its more than 30-year history of innovation, NREL has been a leader in working with green algae for hydrogen and biofuel production, as well as with finding ways to speed renewable fuels to market to help meet the nation's clean energy goals. It is this expertise that encouraged MIT's Iftach Yacoby to partner with NREL, which enabled the researchers to collaborate on technical innovations such as the CdTe-H_2ase.

During NREL's work with green algae, the lab's own Senior Scientist Paul King and other researchers worked with hydrogenase enzymes as a key component of the photosynthetic hydrogen production equation. These biological catalysts can convert electrons and protons into hydrogen gas, or convert hydrogen into electrons and protons. For this work, the team chose to use in vitro tests under anaerobic conditions. They were able to demonstrate how the hydrogenase and other enzymes compete to regulate whether algae uses the solar energy it captures through photosynthesis to produce carbon compounds or hydrogen. As they studied



Photosynthetic electron transport pathways that support carbon dioxide fixation and hydrogen production. Light-activated PSII extracts electrons from water and transfers them, while parallel circuits couple Fd to either FNR for carbon dioxide fixation or hydrogenase production.



Engineering of the hydrogen-producing enzyme to create an Fd-H_2ase fusion changes the composition of the hydrogen production circuit to include both direct (box 1) and indirect (box 2) H_2 production modes. The CO_2 fixation circuit (box 3) remains open, but operates at a reduced level.

these interactions, they were able to devise a procedure to engineer the proteins that compose electron transfer circuits.

The first element of their strategy was based on their hypothesis that they could have more of the electrons go to hydrogen if they altered the composition to replace hydrogenase with a ferredoxin-hydrogenase fusion. In the anaerobic test tubes, the team confirmed that the photosynthetic circuit can switch from capturing carbon dioxide to producing hydrogen by substituting the fusion. The hydrogen production was carried out in the presence of the CO_2 fixation enzyme ferredoxin: NADP-oxidoreductase (FNR). This process is a biological model for using solar power to convert water into hydrogen. The basis for this switch was modeled as two new Fd-hydrogenase circuits (boxes 1 and 2), and a reduced level of FNR activity modeled as a third circuit (box 3).

King considered these results promising, because they suggest that fusion is an engineering strategy to improve hydrogen production efficiencies, and might be useful in resolving the biochemical mechanisms that control photosynthetic electron transport circuits and product levels from competing pathways. The next phase, already underway, is to introduce the fusion protein into green algae Chlamydomonas and determine if rewiring can take place to improve hydrogen-production efficiencies. Even though this is only one of a number of variables to consider, this strategy has already signaled an avenue to pursue in the drive to reduce the cost of hydrogen fuel and make it cost-competitive for industry.

—Ernie Tucker

IMM Solar Cell Shows Its Versatility

Mark Wanlass (left) and Jeffrey Carapella with the metal-organic vapor phase epitaxy deposition system used to grow IMM solar cells.

The IMM cell is both highly efficient and adaptable to many applications.

Inventing a new type of solar cell is one thing. Setting efficiency records with it and winning major awards add to the achievement. But when one of the world's leading manufacturers of compound semiconductor devices likes the technology enough to nurture and develop it for commercial use, that's a line drive straight out of the park.

All of the above applies to NREL's invention of the inverted metamorphic multijunction (IMM) solar cell and the path to commercializing it by RF Micro Devices (RFMD).

The IMM cell is engineered to capture energy from a major portion of the solar spectrum and be both highly efficient and extremely versatile. These capabilities all stem from how the cell is grown—a process that reverses the usual sequence for triple-junction cells because the top layer is deposited first and the bottom layer is deposited last. Then the cell is flipped over, mounted to a "handle" material, such as a thin metal foil, and the substrate that the cell was grown on is removed. One advantage of this approach is that the expensive substrate can potentially be reused, which results in significant cost savings. Another is that because the handle material doesn't need to be crystalline or even a semiconductor, it can be chosen to meet the needs of a particular application.

Triple-junction solar cells such as the IMM are typically used in concentrating photovoltaic devices (CPV), in which lenses and mirrors concentrate the sun's energy to hundreds or thousands of times its normal strength. One problem facing such devices is the buildup of heat. The inverted growth process of the IMM cell makes it easy to add an effective back-surface reflector, which directs any remaining absorbable light energy back into the active subcell layers, where it can be captured and used to boost the cell's overall efficiency. In addition to increasing efficiency, the back-surface reflector rejects the lower-energy infrared radiation, which keeps the cell cooler and allows it to operate more efficiently.

These and other benefits attracted the interest of RFMD, a leading semiconductor manufacturer and telecommunications giant headquartered in Greensboro, North Carolina. Looking to take its expertise in mass-producing semiconductor devices and apply it to the solar energy field, RFMD signed a cooperative research and development agreement (CRADA) with NREL in 2009. NREL scientist John Geisz, one of the key developers of the IMM cell, is the CRADA's principal investigator.

"This entry of the telecom industry into the solar arena is key," said Daniel Friedman, manager of NREL's III-V multijunction device research. "Partnering with the private sector to find new applications for our technologies is important to accelerate the pace of moving energy solutions to the marketplace."

Illustrating this flexibility, in March 2011 RFMD announced the fabrication of dual-junction PV cells that integrate gallium arsenide and indium gallium phosphide PV junctions using the company's existing 6-inch semiconductor equipment. The successful fabrication of the dual-junction PV cells clears the way for RFMD to develop triple-junction structures, with the ultimate goal of developing a commercially viable and high volume-capable compound semiconductor-based process for high-performance PV cells. The conversion efficiency achieved across RFMD's 6-inch wafers was exceptionally uniform, which allows

high device yields and tight distributions in CPV product performance.

"RFMD is very pleased with the world-class performance of our dual-junction cells," said Bob Bruggeworth, president and CEO of RFMD. "With this achievement, RFMD is demonstrating we possess the critical technologies to produce a low-cost PV product with competitive solar cell conversion efficiency, supported by the quality, reliability, and volumes that characterize the cellular handset market."

The IMM technology won an R&D 100 Award in 2008 and a Federal Laboratory Consortium Technology Transfer Award in 2009. It has demonstrated one of the world's highest reported solar cell conversion efficiencies at 40.8%, and research shows that it is likely to continue to substantially improve cell efficiency.

—Susan Moon

Singlet Fission's Two-for-One Potential

NREL scientists confirm an exciting first for singlet fission.

Consumers like to get two-for-one deals. So do scientists at NREL, who are working in collaboration with scientists at the University of Colorado, Boulder and Northwestern University, to search for innovative scientific concepts that may lead to solar cells having very high conversion efficiencies.

Singlet fission is just such a concept, and has the potential to significantly boost our nation's ability to create more abundant and lower-cost solar-generated electricity and hydrogen.

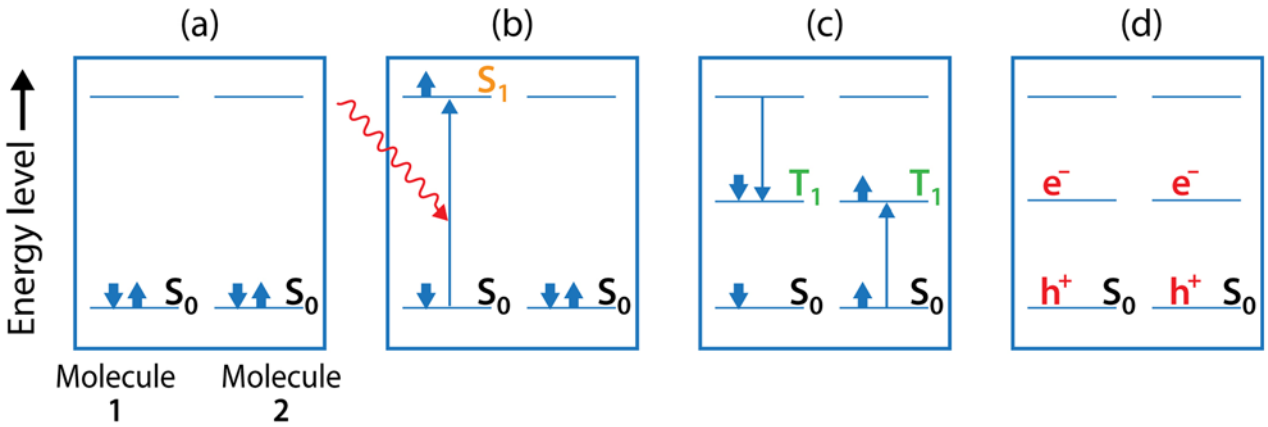
In the fission process, one singlet state excited by a photon of the high-energy portion of sunlight creates two triplet states. In turn, these triplets potentially produce two electron-hole pairs per absorbed photon—the "two-for-one" possibility—in a solar cell, which boosts the energy conversion efficiency.

The collaborating scientists used spectroscopy—on a thin-film of the compound 1,3-diphenylisobenzofuran (DPIBF)—to measure a yield of triplets of 200% (±30%) at a temperature of 77 kelvin. This yield represents nearly perfect efficiency, with two triplets created per one absorbed photon. Also, this result confirms theoretical work that has been conducted on molecules designed with specific properties that favor singlet fission.

Thermodynamic modeling indicates that a simple multilayered solar cell based on singlet fission could increase the photovoltaic power conversion efficiency by more than 43% above the maximum theoretical limit—the so-called Shockley-Queisser limit. The resulting conversion efficiency would be about 46%.

Evolution of a Disruptive Concept

The singlet-fission phenomenon has been known for nearly three decades, but had not been formally considered as a light-harvesting scheme until it was highlighted in a 2006 NREL publication. This work led to an extensive search, guided by principles of quantum mechanics, for appropriate candidate materials. One of these materials, DPIBF, essentially has a perfect ratio of singlet-to-triplet excitation energies of 2 to 1. This means that photons with energy at least twice that of DPIBF's "bandgap" energy can produce two positive and two negative charges, and therefore can potentially double the electrical current of a solar cell.



The basics of singlet fission: (a) Two neighboring organic molecules in their unexcited ground states S_0 (thick arrows indicate electron spin direction); (b) A high-energy photon excites the first molecule, creating a singlet state S_1; (c) The first molecule relaxes to a lower-energy triplet state T_1 and transfers energy to the second coupled molecule, which is excited to a triplet state; (d) The two T_1 states each generate a free electron (e-) and hole (h+). Hence, one photon produces two electron-hole pairs—a two-for-one transaction.

In addition, through their search, NREL researchers and collaborators determined two design principles with promising results. The first identifies a new class of high-potential materials (biradicaloids), and the second establishes a geometry between the two coupled molecules needed for singlet fission that fosters the fission phenomenon. NREL's theoretical, experimental, and characterization work is expanding the potential application of singlet fission to greatly enhance the conversion efficiency of organic-based solar cells.

This concept is an extension of NREL work from the mid 1970s on what are now generally referred to as "third-generation" solar photon conversion approaches. The early work focused on hot-carrier conversion, which is a process in solar cells that increases solar conversion efficiency by using more of the sun's energy rather than losing it as heat. Then, in 2000, an NREL research team identified multiple-exciton generation (MEG) in quantum dots, which are semiconductor nanocrystals that can produce two or more electron-hole pairs (excitons) from one high-energy photon. Singlet fission is the molecular analog of MEG in inorganic quantum dots.

Taking the Concept to the Next Level

The results in singlet-fission research represent a basic science advance by NREL, but it will take much applied research to find ways to use this effect in a commercial solar cell. Singlet fission has been demonstrated spectroscopically to be efficient under the right circumstances. But challenges ahead include understanding how the process functions in a wider range of compounds and how to incorporate these organic molecules into devices.

Consequently, there are probably another ten years of research ahead to prepare these sorts of singlet-fission cells for prime time. Specifically, researchers need to identify optimal materials to use, and then develop these within actual solar devices, with the goal of collecting the electrons produced by the triplet states. The effort will be intense, but the result is that more of the sun's energy will be available to generate solar electricity and produce solar fuels. This is a key step toward making solar electricity and fuels more efficient and cost competitive as a conventional power source.

The research at NREL was sponsored by the Hydrogen Fuel Initiative within the U.S. Department of Energy (DOE) Office of Basic Energy Sciences and that at the University of Colorado and Northwestern University by the Solar Energy Technologies Program within DOE's Office of Energy Efficiency and Renewable Energy.

—Don Gwinner

27-Year R&D 100 Awards Winning Streak

NREL secures three more R&D 100 Awards in 2011.

NREL-developed solar technologies earned three R&D 100 Awards—awards that underscore the lab's leadership among national laboratories in renewable energy and energy efficiency research. Since 1984, NREL has earned 50 of these prestigious prizes.

R&D 100 Awards are considered "the Oscars of Innovation." Each year since 1963, R&D Magazine has identified and recognized revolutionary technologies newly introduced to the market. R&D Magazine editors and a panel of technical consultants, university faculty, and industrial researchers evaluate numerous nominated technologies to select the top 100 technologies based on their potential impact. Past award winners have included the flashcube (1965), halogen lamp (1974), liquid-crystal display (1980), anticancer drug Taxol (1993), and HDTV (1998).

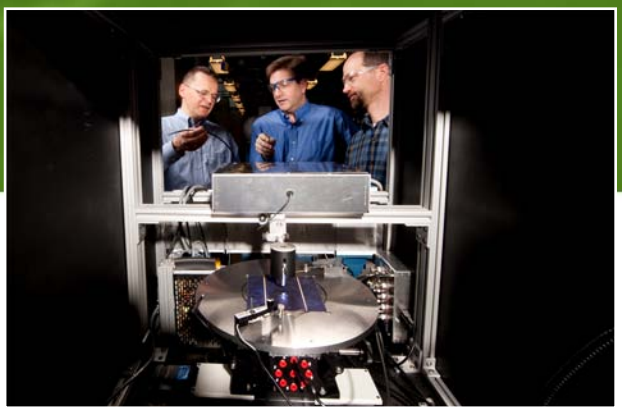
In 2011, NREL and its corporate partners won R&D 100 Awards for the following three technologies.

"Flash" Quantum Efficiency System for Solar Cells

Problem: Solar cell manufacturers want to measure the quantum efficiency (QE) of every cell on a production line. Measurement times, however, have been too slow to evaluate more than a very small sampling.

Solution: NREL's technique, commercialized by Tau Science Corporation, uses a solid-state light source, synchronized electronics, and advanced mathematical analysis to parallel-process QE data in just one second—a rate that is more than 1,000 times faster than the current method.

Impact: At this speed, every cell's QE can be measured on the production line. The results:

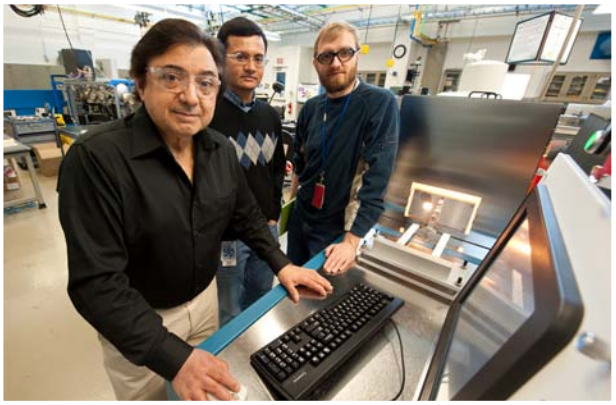


Pauls Stradins, Brian Egaas, and David Young confer behind a prototype of the real-time quantum efficiency system.

- There is real-time quality control of the entire manufacturing process
- QE cells are sorted for optimized power production in modules
- New research and development capabilities now exist, such as mapping QE across an entire cell to help researchers better understand performance).

Optical Cavity Furnace

Problem: Much of the heat generated in industrial furnaces that process solar cells is wasted because it is not focused directly on the cell. Also, the heat is not distributed uniformly across the cell, which leads to sub-par cell performance.



Bhushan Sopori, Vishal Mehta, and Peter Rupnowski at the controls of the Optical Cavity Furnace.

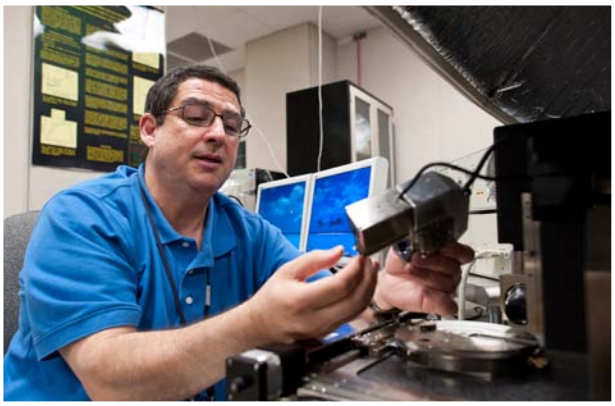
Solution: NREL, working with AOS Solar, Inc., developed an optical cavity design that focuses heat almost entirely on the cell, which tightly controls the heat flux for excellent uniformity across the cell. The light sources for heating have also been designed to allow use of beneficial photonic effects during processing.

Impact: By processing solar cells in the Optical Cavity Furnace, the cells have higher conversion efficiencies than those processed in conventional rapid thermal processing furnaces, and this improved performance occurs at a lower cost.

Silicon Ink for High-Efficiency Solar Cells

Problem: For the solar cell industry to remain competitive, it needs to reduce the cost of crystalline silicon solar cells, but the standard routes for doing this have been exhausted. To accomplish this kind of cost reduction now calls for an entirely different approach.

Solution: Innovalight, a start-up company, invented a liquid form of silicon and came to NREL for expert guidance on optimizing it for use with solar cells. This partnership was a great success, and their work on the technology has resulted in a 1% absolute and 6% relative increase in cell efficiency.



NREL senior scientist Helio Moutinho uses a scanning capacitance microscopy technique to detect signals in solar cells used with Innovalight's Silicon Ink.

Impact: Five of the world's leading solar companies have signed licenses to use Silicon Ink in their production lines. The ink can transform a 35-megawatt (MW) production line into a 37-MW line, which generates additional revenue for cell manufacturers. Given that the technology solution comes at a very low marginal cost, cell manufacturers can boost profitability by as much as 20%.

—Karen Atkison

Carbon Nanotubes for Batteries

Groundbreaking battery technology holds potential to revolutionize powering vehicles.

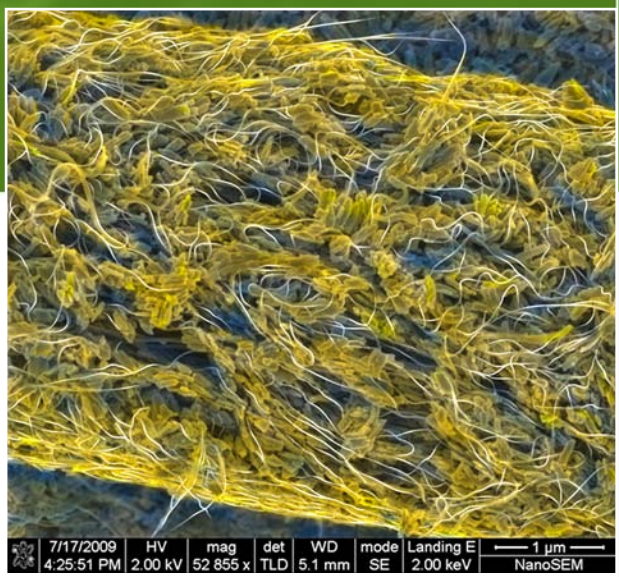
At about one ten-thousandth the size of a human hair, carbon nanotubes may be miniscule, but they are also mighty. Corral a few billion of them, and their powerful energy-related applications can impact solar cells, wind turbine blades, and batteries.

Materials used for capturing solar and wind energy have long and successful research histories at NREL. Now that success also applies to materials used in batteries.

This happened recently when NREL scientists revealed their groundbreaking findings on metal oxide nanoparticles as high-capacity anode materials. They expanded on that research by employing carbon nanotubes to enhance the performance of batteries. Senior Scientist Anne Dillon leads this effort, which began about 4 years ago.

The goal of the nanotube research was to use carbon nanotubes as the "conductive additive" in electrodes for lithium-ion batteries designed for next-generation vehicles. It was essential that the component materials be inexpensive, nontoxic, and durable—and that the electrode have a high charge/discharge rate and a high reversible capacity. The NREL team accomplished just that by using the properties of long carbon nanotubes with a highly crystalline structure in a two-step process that synthesized nanoparticles of an oxide of iron (Fe_3O_4) embedded in a "nanotube net." The net can maintain electrical conductivity without a polymer binder, an improvement that enhances the space for active materials in this new electrode to 95% (compared to about 80% for typical electrodes). Better yet, the binder-free electrode is both stable and has a high reversible capacity.

Having achieved this, the scientists moved on to researching the cathode—with equally successful results. They demonstrated that the nanotube net improves conductivity and stabilizes the surface



This color-enhanced cross sectional image shows the Fe3O4 nanorods (yellow/blue) and 5 wt % carbon nanotubes (white).

with an astonishing 6-minute charge/discharge rate. This study included the collaboration of Professor M. Stanley Whittingham of the State University of New York at Binghamton, who is widely recognized as the inventor of lithium-ion batteries.

So far, this research has produced one patent and two high-impact articles in *Advanced Energy Materials*. The two articles were highlighted in "Materials Views" and one made the publication's cover. The NREL research team also made the strategic move of hiring Chunmei Ban, a gifted young scientist. She was a graduate student in the Whittingham group when she came to NREL for a 2-year postdoctoral position. Such was the value of her contribution to this project that she was hired on staff.

Dillon credits the rapid achievements to many things. One is NREL's Laboratory Directed Research and Development (LDRD) program, which backed the first year of research based on the project's innovative concept and considerable upside potential. LDRD projects provide an important mechanism to establish proof of principle of new, innovative concepts.

Another key to advancement is NREL's core expertise in related technologies such as electrochromic windows, which are similar to batteries. Perhaps even more important is NREL's ambience. "We have the facilities we need, a

collaborative environment, and a mindset to accomplish things," says Dillon.

This groundbreaking battery technology is currently available for licensing. Potential investors may be concerned that it is too costly based on the necessity of using lasers to produce the nanotubes, but Dillon points out cost advantages related to longer lifetimes and savings on materials. "Our back-of-the-envelope calculations indicate that it may cheaper in the end," she says.

—*Susan Moon*

Dan Says continued...

applied R&D begins. Each step informs the other; it all works together.

The field of biofuels is a great example of how this works in practice. Our first relatively crude forays into turning plants into fuel were based on centuries of knowledge about how to make beer and wine. We used those lessons of fermenting to make alcohol fuels, such as ethanol. Today, we're applying modern approaches such as electron microscopes, advanced computer modeling, and other tools of basic science to truly understand the incredibly complex processes at work. These insights allow us to develop new technologies that produce energy-rich hydrocarbons that closely mimic fossil fuels, such as gasoline, but do so using renewable, sustainable, and environmentally-friendly biomass resources. Read more about this in "Better Biofuels through Computational Analysis."

The overarching question is how to best marshal national resources to surmount our most critical energy challenges. As a member of the Advisory Board of the Energy Research, Development, & Deployment Policy Project (ERD3) at the Harvard Kennedy School's Belfer Center for Science and International Affairs, I have seen first-hand that all models of research do not produce equal results. The ERD3 Project's just-released study, "Transforming U.S. Energy Innovation," found that to achieve our national goals, energy innovation will require a clearly defined mission, exceptional managerial talent with proven technical expertise, much stronger partnerships between federal researchers and private industry, and finally, world-class research institutions supported with consistent and sufficient public funding. We look forward to working with the U.S. Department of Energy and our many stakeholders to put such findings to good use.

At NREL, we are proud of our comprehensive, integrated, and deliberate approach to clean energy R&D. But the more I've learned about how to produce valuable new technologies—and do so in the best, fastest, and most cost-effective ways possible—the less I'm truly surprised. After all, hasn't necessity always been the mother of invention?

Dr. Dan E. Arvizu
Director
National Renewable Energy Laboratory

About

Continuum Magazine is NREL's quarterly publication that showcases the laboratory's latest and most impactful clean enaergy innovations and the researchers and unique facilities that make it all happen.

Editorial Staff

Kim Adams, Managing Editor
Bill Gillies, Creative Director
Jennifer Josey, Web Project Manager
Rebecca McEwen, Print Editor
Michael Oakley, Web Developer
Kristin Tromly, Web Content Strategist

Editorial Board

Heidi Blakley, Anya Breitenbach, Michelle Kubik, Heather Lammers, and Susan Moon

Design

Media Fusion

Image Credits:

Front cover image courtesy BioMed Central, originally published January 26, 2011, in the article, In planta expression of A. cellulolyticus Cel5A endocellulase reduces cell wall recalcitrance in tobacco and maize by Roman Brunecky, Michael J Selig, Todd B Vinzant, Michael E Himmel, David Lee, Michael J Blaylock and Stephen R Decker; front cover first inset photo courtesy of Sandia National Laboratories; front cover second inset image by NREL; front cover third inset image by NREL; inside front cover photo by Dennis Schroeder, PIX 19386; page 1, first inset image by NREL; page 1, second inset image by NREL; third inset photo courtesy of Sandia National Laboratories; page 2 image by NREL; page 3 illustration by NREL; page 4 illustration by NREL; page 6 image by Matthew Churchfield and Kenny Gruchalla/NREL; page 7 photo by Dennis Schroeder, PIX 19886; page 8 image by Ross Larsen and Kenny Gruchalla/NREL; page 10 photo courtesy of Sandia National Laboratories; page 11 photo by Dennis Schroeder, PIX 20068; page 12 photo courtesy of Sandia National Laboratories; page 13 illustration by John Perkins/NREL; page 14 photo courtesy SLAC National Accelerator Laboratory; page 15 photo by Dennis Schroeder, PIX 18850; page 15 and 16 illustrations by Paul King/NREL; page 17 photo by Pat Corkery, PIX 15934; page 19 illustration by NREL; page 21, first photo by Dennis Schroeder, PIX 19542; page 21, second photo by Dennis Schroeder, PIX 19518; page 22 photo by Dennis Schroeder, PIX 19556; page 23 image by NREL.

National Renewable Energy Laboratory
1617 Cole Boulevard, Golden, Colorado 80401-3305
303-275-3000 • www.nrel.gov

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency and Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

NREL/BK-6A42-53932 • February 2012

Printed with a renewable-source ink on paper containing at least
50% wastepaper, including 10% post consumer waste.