




**NREL** National Renewable Energy Laboratory

A national laboratory of the U.S. Department of Energy  
Office of Energy Efficiency & Renewable Energy

*Innovation for Our Energy Future*

A 3D molecular model of a crystal lattice structure, likely silicon, rendered in shades of blue and grey. The atoms are represented as spheres, and the bonds as rods. The model is set against a dark background with glowing blue and red lines, suggesting energy or data flow.

*National Renewable Energy Laboratory*  
**2003 Research Review**

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## feature



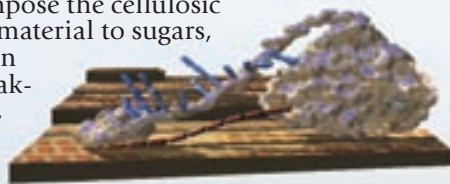
## 2 New Horizons for Hydrogen

*Aspects of a hydrogen future:* The cover shows a photoelectrochemical cell that uses sunlight to produce hydrogen from water; a hydrogenase enzyme from the green alga *Chlamydomonas reinhardtii* that catalyzes the release of hydrogen gas from water; and a single-wall carbon nanotube, which offers the promise of a safe and reliable way to store hydrogen.

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### 10 Unraveling the Structure of Plant Life

Cellulase enzymes may be used to decompose the cellulosic fiber in plant material to sugars, which can then be used for making chemicals, fuels, materials, and other products.



### 16 Winds of Change

By 2020, carbon dioxide emissions from power plants in the United States are expected to increase by nearly 50%. But much of this increase could be offset if the use of wind energy were to continue its rapid growth and gain a significant share of the electricity market by 2020.



## departments

**1 Perspective** NREL's R&D in hydrogen and other areas of renewable energy and energy efficiency will help our nation diversify its energy supply and power its economy, and will benefit its environment.

**20 Awards & Honors** NREL wins four R&D 100 awards, two FLC technology transfer awards, and welcomes a new fellow of the American Association for the Advancement of Science.



**22 NREL in Focus** The Laboratory names a new research fellow, selects a director for the bioenergy center, assumes the role for integrating hydrogen systems, plans a new R&D facility, and builds computing capability.

**25 Patents** Nineteen new NREL technologies are patented, ranging from electrochromic and photoconductive materials to thin-film photovoltaics to ethanol production.

**The NREL Research Review.** The National Renewable Energy Laboratory is operated by Midwest Research Institute and Battelle for the Department of Energy's Office of Energy Efficiency and Renewable Energy. NREL is the nation's premier laboratory for R&D on renewable energy and a leading laboratory for energy efficiency. The *Research Review* is published yearly and describes the Laboratory's accomplishments in science and technology to a wide audience. The purpose is not simply to describe the progress being made, but also to show the promise and value of NREL's R&D to people, industry, the nation, and the world.

# Perspective

## Pursuing the Goal

NREL's focus on science and technology, from innovation to implementation, is to make abundant energy available to all people with minimal adverse effects on our environment. This 2003 edition of the *NREL Research Review* highlights some of the technology development advances we have made toward that goal, beginning with the production of hydrogen from renewable sources. NREL scientists made important strides in methods including the gasification and pyrolysis of biomass, electrolysis of water using electricity produced by wind and other renewable energy technologies, and direct water-splitting via photoelectrochemical and photobiological techniques. (See "New Horizons for Hydrogen," page 2.)

In biomass research, NREL worked with industry to engineer enzymes that are more efficient at breaking down cellulose into sugars, culminating in a 12-fold reduction in the cost of enzymes. (See "Unraveling the Structure of Plant Life," page 10.) Researchers also determined how to increase the amount of solids that could be tolerated in slurries while producing sugars from biomass, which will markedly reduce the cost of bio-based fuels, chemicals, and other products.

NREL took another step forward in 2003 toward the goal of cheaper, more reliable wind power by developing a capability to test industry's wind turbine blades at their natural resonant frequency along two axes of the blade. This enables researchers to assess a wide range of larger blades for their tendency toward fatigue and delamination. As one of the most rapidly growing renewable electricity technologies,

wind energy is a critical technology in offsetting carbon dioxide emissions that contribute to global warming. (See "Winds of Change," page 16.)



**Dr. Stanley R. Bull, Associate Director, Science & Technology**

Photovoltaics is also a vital technology that will reduce carbon dioxide emissions from conventional electricity production. NREL researchers and their industry partners recently set five conversion efficiency records, one involving the world's most efficient cell design — a triple-junction GaInP<sub>2</sub>/GaAs/Ge cell that converts 36.9% of solar energy to electricity under a

concentration of 309 suns. As another example, thin-film cells have reached efficiencies of 19.2%, a performance similar to standard multicrystalline silicon cells. These lab-scale advances will ultimately help lower the cost of commercial-scale solar modules.

In the area of advanced vehicle and fuel technologies to reduce our dependence on foreign oil, NREL has licensed its simulation software — ADVISOR — to AVL Group, a company that develops power trains and advanced vehicle simulation technologies. ADVISOR is a modeling tool that helps automakers design fuel cell and hybrid power trains for optimum vehicle performance, economy, and emissions; and already has an established user community of several thousand users.

In buildings energy research, NREL scientists developed software — *BEopt* — that enables engineers, architects, and others to choose the best materials and designs to minimize building energy use and costs for any given climate and location. The software also shows the most effective and least costly path toward designing buildings that could achieve zero net energy use.

NREL is in the forefront of the developments needed to bring distribut-

ed generation of electricity into the marketplace, which will benefit not only individual buildings but also industrial plants, communities, and other localized electrical loads. Working with industry and utilities, NREL researchers led the effort to develop and win approval for new uniform national standards for the interconnection of distributed generation technologies. These standards will enable the interconnection of distributed generation systems of various types to the electrical grid, other distributed systems, and individual loads, helping to improve power reliability and quality while improving the environment.

The foundation of all this work is our basic understanding of the materials and fundamental mechanisms related to these technologies. In 2003, nanosciences made important advances at NREL. Scientists are using self-assembling proteins — bacterial cellulosomes — to organize III-V semiconductor quantum dots into arrays, with eventual applications in high-efficiency solar cells, solid-state lighting, and lasers. NREL also made significant progress in understanding and developing carbon nanotube structures that can store effective amounts of hydrogen in a lightweight device for future use in fuel-cell vehicles.

Computational science is becoming an equal partner with experimental and theoretical science (see page 24). NREL scientists are simulating the diffusion of oxygen and hydrogen in algal hydrogenase, which will guide genetic modification of the algae and optimize production of hydrogen. Researchers are also simulating the fluid and thermal dynamics of spray cooling to study the application of this technique to automotive electronics, condensers at geothermal power plants, and other areas. With research applications multiplying rapidly, we will continue to build our capability in this critical methodology.

As exciting as these advances have been in 2003, much remains to be done. We look forward to both steady progress and important breakthroughs as we keep pursuing the goal in 2004.



# New Horizons For Hydrogen

## Producing Hydrogen from Renewable Resources

These days, you'll likely notice the buzz about hydrogen and fuel cells — in conversations at local coffee shops, in newsstand headlines, and on the nightly news report. The president's Hydrogen Fuel Initiative, unveiled in his January 2003 State of the Union address, has captured the nation's attention by highlighting the possibility of a clean and sustainable energy future based on hydrogen. This vision of a new hydrogen economy "will mean a world where our pollution problems are solved and where our need for abundant and affordable energy is secure... and where concerns about dwindling resources are a thing of the past." -- Spencer Abraham, *Hydrogen Energy Roadmap*, November 2003.

### Renewable Hydrogen

Hydrogen is the most abundant element in the universe. And while it doesn't exist by itself on Earth, it can be produced from a wide variety of resources — coal, oil, natural gas, biomass, and water. This versatility contributes to the promise of hydrogen, allowing it to be produced where and when we need it.

About 95% of the hydrogen we use today comes from reforming natural gas. The remainder, high-purity hydrogen from water electrolysis, is primarily produced using electricity generated by burning fossil fuels. But to realize the full benefits of a hydrogen economy — sustainability, increased energy security, diverse energy supply, reduced air pollution and greenhouse gas emissions — hydrogen must be produced cleanly, efficiently, and affordably from domestically available renewable resources.

The ultimate goal is a sustainable cycle of hydrogen production and use. In the first stage of the cycle, hydrogen is produced from renewable resources, such as via photoelectrolysis of water, in which energy from the sun is used to convert water into hydrogen and oxygen. The hydrogen is then used to power a fuel cell, in which hydrogen and oxygen from air recombine to produce electricity, heat, and water. This cycle produces no pollution and no greenhouse gases. Advanced technologies that produce renewable hydrogen as part of this cycle will play a leading role in the future hydrogen economy.

NREL explores several options for producing hydrogen from renewable resources, including biomass conversion; electrolysis using electricity from renewable resources, in particular from wind energy; and direct water-splitting using microorganisms or semiconductors. Some technologies are ready for real-world demonstrations. Others are just emerging and will require long-term R&D investment. But all are focused on the same goal — producing clean, sustainable hydrogen.

### Hydrogen from Biomass

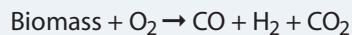
Since the Laboratory opened in 1978, NREL has been developing methods for converting biomass to fuels, chemicals, heat, and power. Building on the successes of these efforts, biomass is now one of the best near-term options for producing renewable hydrogen.

Biomass resources are abundant and widely distributed throughout the United States. And because biomass consumes atmospheric carbon dioxide (CO<sub>2</sub>) during growth, it can have a small net CO<sub>2</sub> impact compared with fossil fuels, effectively sequestering carbon and reducing our nation's greenhouse gas emissions.

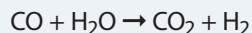
Biomass feedstocks like agricultural and forest residues, consumer wastes, and crops specifically grown for energy production are composed of three interconnected polymeric materials — cellulose, hemicellulose, and lignin. Of the technologies used to break down this biomass structure and produce hydrogen, perhaps the ones closest to being competitive with conventional means are the thermochemical processes of gasification and pyrolysis.

**Gasification** is a two-step process in which biomass is thermochemically converted into a combustible gas. In the first step, the volatile components of the fuel are vaporized (in the presence of oxygen, air, or steam) at temperatures below 600°C by a set of complex reactions. This yields a mixture of CO<sub>2</sub>, carbon monoxide (CO), tar,

hydrogen (H<sub>2</sub>), and water vapor (H<sub>2</sub>O), with by-products of char and ash. In the second step, the char is gasified at 800°–850°C through reactions with oxygen (O<sub>2</sub>), steam, and H<sub>2</sub>. This yields a mixture of gases that primarily consists of CO, CO<sub>2</sub>, and H<sub>2</sub>. Some of the unburned char is combusted to provide the heat needed for the gasification. The overall reaction is:



The gas product of this process requires conditioning to remove tars and inorganic impurities. Carbon monoxide is converted to additional hydrogen by the water-gas-shift reaction:

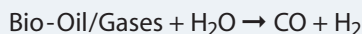


**Pyrolysis** is a process that thermally degrades biomass to a mixture of gases, char, and an oxygen-rich liquid called bio-oil. Pyrolysis takes place at 500°–800°C in the absence of oxygen. The overall reaction is:

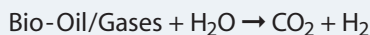


The relative proportions of the three products depend on the pyrolysis method, the characteristics of the biomass, and the reaction conditions — heating rate, temperature, and residence time. For example, pyrolysis has been used to produce charcoal for centuries. This requires relatively slow reaction rates at very low temperatures to maximize solid yield. Fast pyrolysis is used to maximize either the gas or liquid products, depending on the temperature employed.

The bio-oil and gases are converted to hydrogen using catalytic steam reforming, followed by the water-gas-shift reaction. The catalytic steam reforming reaction takes place at 750°–850°C over a nickel-based catalyst:

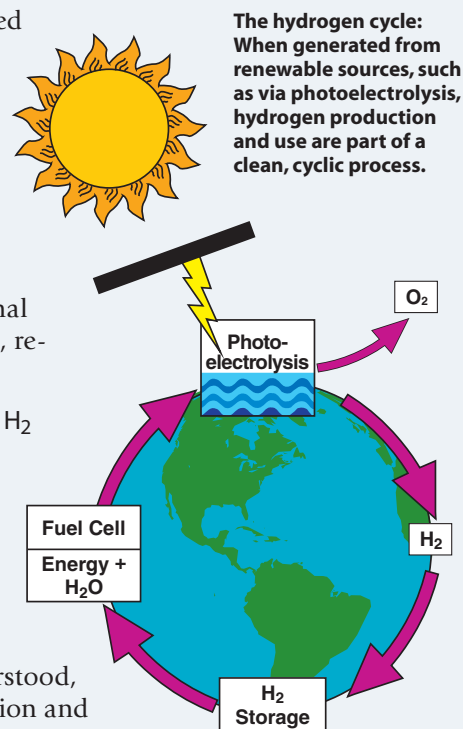


The CO is converted into additional H<sub>2</sub> by the water-gas-shift reaction, resulting in the overall reaction:



As the final step in both gasification and pyrolysis, the H<sub>2</sub> and CO<sub>2</sub> are separated to yield H<sub>2</sub> that is 99.99% pure, meeting the requirements for use in a fuel cell.

**Co-products.** Although well understood, the processes of biomass gasification and pyrolysis face challenges. To be competitive,



**The hydrogen cycle:** When generated from renewable sources, such as via photoelectrolysis, hydrogen production and use are part of a clean, cyclic process.

#### Biomass Resource Potential

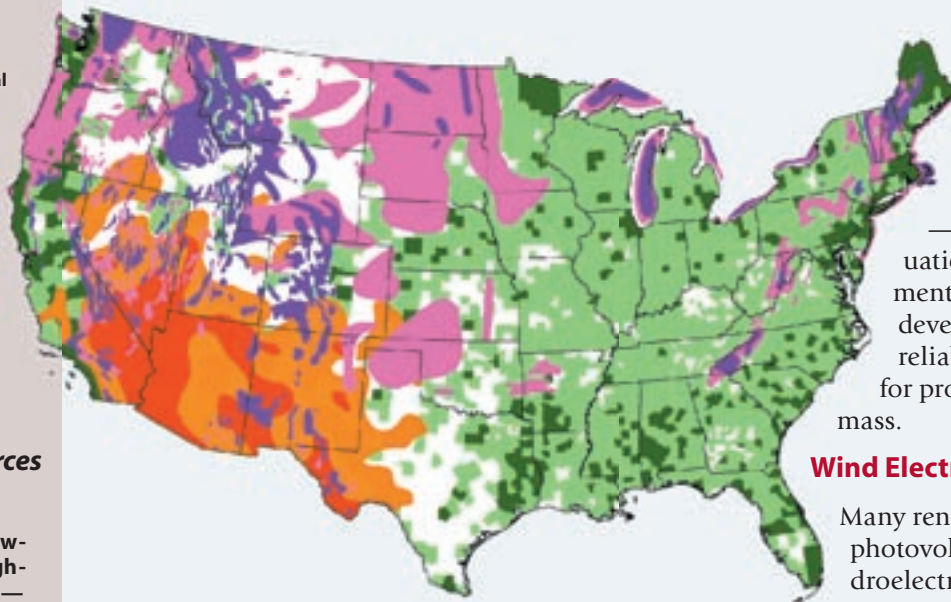
Excellent  
Good

#### Concentrating Solar Power Resource Potential

Excellent  
Good

#### Wind Resource Potential

Excellent  
Good



### Renewable Resources for Hydrogen

We have enough renewable resources throughout the United States — from wind, solar, biomass, etc. — to meet the energy needs of the entire country. The wide distribution of renewable resources allows the use of decentralized hydrogen production from coast to coast. For example, in Iowa, hydrogen could be produced as a byproduct of the corn ethanol production process; and in Massachusetts, it could be produced from electricity generated by off-shore wind farms. Decentralized hydrogen production using renewable resources available regionally reduces or eliminates the cost associated with hydrogen storage and delivery. (Storage is a major challenge, however — see sidebar “Storing Hydrogen in Carbon Nanotubes,” page 8.)

higher process efficiencies and better heat and mass integration are needed. The processes must be flexible enough to handle a range of low-cost feedstocks and their variations in chemical and physical characteristics. Large-scale technology demonstrations of the entire biomass-to-hydrogen process are needed to optimize the process and prove its viability. Plus, we must be able to derive other valuable products from biomass.

This is where pyrolysis has an advantage over gasification. Because bio-oil is made up of two distinct fractions, it can be separated based on water solubility. The water-soluble fraction can be converted to hydrogen via catalytic steam reforming, and the water insoluble fraction can be used to make high-value adhesives. While this approach is not yet cost-competitive, it remains a long-term strategy for converting biomass to hydrogen. Meanwhile, NREL is investigating other coproduct opportunities.

**Other feedstocks.** In the lab, researchers are evaluating low-cost, potentially high-yield renewable feedstocks — agricultural residues, mixed plastics, trap grease, textiles, and other organic materials in the post-consumer waste stream — for their potential to produce hydrogen using pyrolysis/steam-reforming technology.

**New catalysts.** Scientists are designing cost-effective, feedstock-flexible reforming catalysts. Commercially available catalysts cannot withstand the harsh conditions required to produce hydrogen from pyrolysis liquids, resulting in catalyst losses of 10%–20% by weight per day. NREL has developed new nickel-based catalysts to withstand reaction conditions. Testing on pyrolysis oils from pine and mixed hardwoods verified that the new catalysts can produce hydrogen with efficiencies as good as or better than those of the best commercial catalysts. These cata-

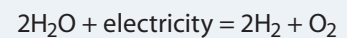
lysts are being modified for use with other feedstocks.

All of these investigations — co-products, feedstock evaluation, and catalyst development — are contributing to the development of an optimized, reliable, cost-effective process for producing hydrogen from biomass.

### Wind Electrolysis

Many renewable technologies — photovoltaics, wind, biomass, hydroelectric, and geothermal — can generate the clean and sustainable electricity needed to run an electrolyzer. But for electrolytic hydrogen production to be cost-effective, we need a low-cost source of renewable electricity. During the past 25 years, advances in wind turbine technology have dramatically reduced the cost of wind power. Today, the cost of wind electricity typically ranges from 3–7¢/kWh for utility-scale projects. This puts wind electrolysis in a good position to be the first economical renewable hydrogen-production system.

In wind electrolysis, the wind turns the blades of a wind turbine, and the blades spin a shaft, which connects to a generator to make electricity. An electrolyzer uses this electricity to separate water into hydrogen and oxygen:



Proton exchange membrane (PEM) electrolyzers, which are being investigated for this application, consist of a membrane sandwiched between two catalyst-coated electrode plates. At the positively charged electrode (anode), water is split into protons ( $\text{H}^+$ ), electrons ( $e^-$ ), and oxygen. The oxygen is collected or released, and the electrons move through an external circuit under the influence of an applied electric field. The protons move through the membrane and combine with electrons at the negatively charged electrode (cathode) to form  $\text{H}_2$ .

Producing both electricity and hydrogen from wind turbines offers the promise of optimizing electrolysis and power-system efficiencies and lowering costs. For example, producing hydrogen with wind power can improve the ability to dispatch electricity when needed, which is a limitation associated with the intermittent nature of wind energy. When the wind turbine is producing electricity, hydrogen can be produced via electrolysis and stored for later use. The stored hydrogen can then be used in a fuel cell

to produce electricity during times of low power production or during peak demand.

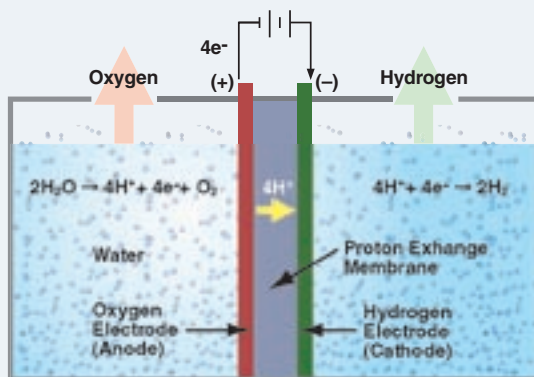
Coupling wind turbines with low-cost electrolyzers can also reduce the cost of a system by minimizing redundancy. For example, variable speed wind turbines rely on power electronics to convert the “wild AC” (variable frequency, variable voltage) produced at the generator to DC, which, when connected to the grid must be converted back to AC at grid frequency (60 Hz). Electrolyzers designed for grid-connected operation also incorporate power electronics to convert AC from the grid to DC power required by the electrolyzer cell stack. These power converters represent a significant percentage of the total cost of the wind turbine and electrolyzer.

To make wind electrolysis cost-effective, researchers will have to lower the cost of wind electricity itself, design more efficient electrolyzers, and optimize the wind/electrolyzer integrated system. Once they’ve done this, they will still need to resolve the logistics of integrating wind electrolyzer systems with utility systems at local, regional, and national levels.

One step toward meeting these challenges is a planned demonstration of integrated electrolysis systems at NREL’s Wind Hybrid Test Facility. For this demonstration, NREL is designing a single power-electronics package and controller that will eliminate redundancy in the wind electrolysis system and allow the power output of wind turbines to match the power requirements of electrolyzers. Success here will help pave the way for commercializing the concept.

## Direct Hydrogen Production

Direct water-splitting technologies — using photoelectrochemical devices or photosynthetic microorganisms — are the “Holy Grail” of the hydrogen economy. These processes use



In a PEM electrolyzer cell, water is split into protons (H<sup>+</sup>), electrons (e<sup>-</sup>) and O<sub>2</sub> at the anode. The protons move through the membrane to the cathode, where they combine with electrons to form H<sub>2</sub>.

energy from sunlight to dissociate water into hydrogen and oxygen. They are the ultimate clean and sustainable hydrogen production methods. Although not ready for prime time, photoelectrochemical and photobiological technologies show great promise for the future and are the focus of long-term R&D efforts at NREL.

**Photoelectrochemical research.** A photoelectrochemical (PEC) hydrogen system integrates photovoltaic (PV) material with an electrolyzer to produce hydrogen directly from water, using only sunlight. This system offers many benefits over two-step processes in which the PV cells and electrolyzer are separate components of the system. Combining the two components in a single PEC device can eliminate most of the electrolyzer costs and reduce semiconductor processing because surface contacts, interconnects, and wiring are no longer necessary. It can also increase the efficiency of the process by 30%, further reducing the cost of delivered hydrogen.

The basic PEC hydrogen production system consists of two electrodes — a semiconductor electrode and a platinum metal electrode — immersed in an aqueous electrolyte. But instead of using electricity from an external source like wind power, the semiconductor absorbs light energy and generates the electrical current that drives the electrolysis reaction, splitting water into hydrogen at the semiconductor surface and oxygen at the metal electrode surface.

Although simple in concept, the challenge is to find a material that can drive this one-step process. For it to be viable, two criteria must be met — the light-harvesting system must have the correct energetics to drive the electrolysis, and the system must be stable in an aqueous environment (see sidebar “The Right Energetics,” page 6).

So far, no single semiconductor has been identified that satisfies all of the criteria for use in a hydrogen-evolving PEC system. The most stable semiconductors in aqueous solution are oxides, but their band gaps are too large for efficient light absorption, or their semiconductor characteristics are poor. Semiconductors with better solid-state characteristics are typically thermodynamically unstable with respect to oxidation.

Finding a material that can drive the process is the key to the success of PEC hydrogen production. Materials now under evaluation — gallium nitrides, amorphous silicon, and copper indium gallium diselenide films (CIGS) — build on materials developed for PV. A variety of surface treatments — protective coatings and band-engineering — are also being evaluated to

address energetic issues, corrosion problems, and catalysts for the water-splitting reactions.

Gallium nitrides, although expensive, are good candidates for PEC hydrogen systems because they show high efficiencies, are chemically stable, and their band gaps can be adjusted by altering their composition to produce alloys of gallium nitride. Gallium phosphide nitride and indium gallium nitride are being evaluated to determine if they can be tailored to meet the requirements for solar water-splitting.

Amorphous silicon (a-Si) multijunction systems developed for PV offer a lower-cost alternative to gallium nitride materials. Triple-junction a-Si devices have voltages sufficient for water splitting, and the cells can be tailored to produce voltages matched to the energetic requirements of water-splitting, maximizing overall efficiency. But a-Si is unstable in aqueous solutions and must be protected by a corrosion-resistant coating in a PEC-hydrogen system. To maintain the

function of the semiconductor, the coating material must be stable, transparent, and conductive. For this, researchers are evaluating silicon nitride compositions.

Semiconductor materials based on polycrystalline thin films, such as CIGS, are also promising alternatives. They are made with inexpensive techniques and can reach efficiencies greater than 15%, both of which help reduce costs. Incorporating sulfur into CIGS increases the band gap into the range required for PEC water-splitting. Making a viable CIGS water-splitting device would greatly decrease PEC hydrogen production costs.

Once we identify a semiconductor material with the ideal band gap and chemical stability, it still won't split water unless the semiconductor band edges overlap the water redox potential. This energetic mismatch can be overcome by using a tandem semiconductor system or by modifying the semiconductor band edges. NREL researchers

have demonstrated a solar-to-hydrogen conversion efficiency of 12.4% using a unique structure based on a gallium indium phosphide/gallium arsenide (GaInP<sub>2</sub>/GaAs) tandem system. In this configuration, the GaAs cell generates the additional voltage needed to overcome the energetic mismatch between the GaInP<sub>2</sub> semiconductor and the water redox reactions. Researchers are investi-

NREL scientist John Turner demonstrates the ability of a PEC cell to produce hydrogen from water using energy from a light source.



### The Right Energetics

For a PEC-hydrogen structure, system energetics are a function of the intrinsic electronic properties of the semiconductor material and the electrochemistry at the interface of the semiconductor and the electrolyte.

According to the band theory of solids, which describes the electrical conductivity of solid materials, the available energy levels for electrons in a material form two bands — a valence band and a conduction band. The energy difference between the two bands is called the band gap energy. When a semiconductor absorbs light (photon) energy, electrons from the valence band are excited into the conduction band to generate a current. Only photons with energy equal to or greater than the band gap of the material

can free an electron from the valence band to the conduction band. To absorb a large portion of the solar spectrum, the band gap must be less than 2.2 electron volts (eV). For PEC applications, the electrical output must also be large enough to drive the water-splitting reaction (greater than 1.23 eV). The ideal material for a PEC-hydrogen system has a band gap of 1.6–2.2 eV.

In a PV system, a solid-state junction is the active layer where charge transfer occurs. In a PEC system, the interface between the semiconductor and the electrolyte is the active layer. The characteristics of the band edges (i.e., the top edge of the valence band and the bottom edge of the conduction band) at this interface determine whether water splitting takes place. For a given semiconductor material, the energetic positions of the bands at the semiconduc-



gating the effects of adsorption of organometallic compounds on the band-edge properties of GaInP<sub>2</sub>. In theory, these materials should shift the band edges into the water-splitting range, and speed up the charge transfer rate at the surface. Understanding and controlling the interfacial properties of semiconductor electrodes is key to successfully producing hydrogen from PEC systems.

The development and characterization of new semiconducting materials and systems are critical for the future viability of PEC-driven hydrogen generation. Continuation of the collaborative relationship between PV and PEC hydrogen R&D will accelerate progress in identifying and synthesizing more efficient, lower-cost, and electrochemically stable solid-state materials and systems.

**Photobiological research.** The green alga, *Chlamydomonas reinhardtii*, is one of several microorganisms that uses sunlight to produce hydrogen directly from water. Like all green plants, this green alga also produces oxygen during photosynthesis. Unfortunately, oxygen inhibits the function of algal hydrogenase, the enzyme in *Chlamydomonas* that catalyzes the release of hydrogen gas. So under normal conditions, i.e., in sunlight, the alga cannot sustain hydrogen production for more than a few minutes.

Before photobiological hydrogen production can become a viable commercial-scale option, scientists need to find ways to control the oxygen sensitivity of the hydrogenase. Researchers are attacking this problem on two fronts — by isolating new forms of the organism that can sustain hydrogen production in the presence of oxygen and by developing processes that separate the oxygen and hydrogen production reactions in the algae.

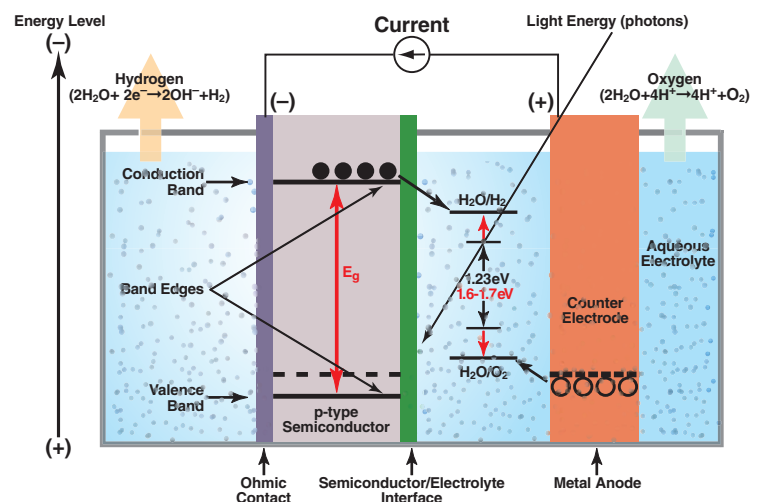
In the first approach, researchers are using advanced molecular engineering to design hydrogenase enzymes that are more resistant to oxygen inactivation. Past research indicates that the oxygen inactivation occurs when oxygen binds directly to one of the iron species located at the catalytic center of the enzyme. Researchers developed a model of the hydrogenase structure to help identify regions in the enzyme most likely to be involved in access of oxygen to the catalytic site. This led to the discovery that the gas channel, which allows hydrogen to diffuse out of the catalytic center of the enzyme, is large enough to allow oxygen to flow back into the catalytic site and deactivate the enzyme. Researchers inserted bulky amino acid molecules along the gas channel walls to reduce the size of the channel so that hydrogen, but not oxygen, could flow through it. This modified enzyme appears more resistant to oxygen deactivation than the original. Researchers are continuing this molecular engineering approach to further improve oxygen tolerance of the alga.

In the second approach, researchers are identifying and characterizing the process conditions that allow the algae to produce either oxygen or hydrogen, but not both simultaneously. They designed a metabolic switch to cycle algal cells between a photosynthetic growth phase, which produces oxygen, and a hydrogen production phase. The switch is based on withholding sulfur, essential for maintaining normal photosynthesis; without it, the algae decrease their photosynthetic activities to low levels (such that any oxygen evolved is immediately consumed by the respiratory activity of the culture) and become anaerobic in the light. As a consequence, they switch to a different metabolic pathway — one that utilizes the reductants generated by water oxidation — to produce hydrogen gas instead. This pathway, which involves a

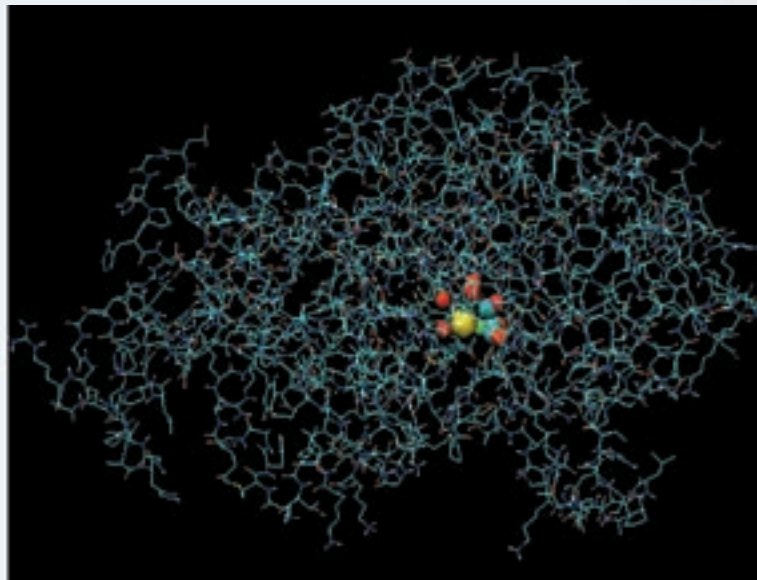
**In a PEC hydrogen system, a semiconductor cell and a platinum metal electrode are immersed in an aqueous electrolyte. The semiconductor absorbs light energy to generate the current that drives the electrolytic reaction, with hydrogen produced at the semiconductor electrode and oxygen at the metal electrode. For this configuration to work, the band gap of the semiconductor must be between 1.6 eV and 2.2 eV, the band edges must straddle the water redox potential, the system must be stable in solution, and charge must be transferred quickly from the semiconductor surface to the water.**

tor surface are fixed. For water splitting to occur, the band edges must overlap the energy levels of the hydrogen- and oxygen-evolving reactions (the water oxidation-reduction potential). Specifically, the conduction band edge must be higher in energy than the hydrogen-evolving half reaction (-0.41 eV), and the valence band edge must be lower in energy than the oxygen-evolving half reaction (0.82 eV).

In addition, charge transfer from the semiconductor surface to the water must occur quickly. If electrons build up on the surface of the semiconductor, they shift the band edges in a negative direction and possibly out of the range required for water-splitting. To accommodate this possibility, band-edge characteristics can be shifted to the required energetic positions through chemical modification of the semiconductor electrode surface.



**Structural model of the hydrogenase enzyme from the green alga *Chlamydomonas reinhardtii*.** The different colored lines depict individual atoms that constitute the enzyme: dark blue for nitrogen, red for oxygen, white for hydrogen, yellow for sulfur, and light blue for carbon. The catalytic center for the hydrogenase — the portion of the enzyme that synthesizes hydrogen gas — is depicted in ball form, showing atoms of iron (green) and sulfur, along with carbon, nitrogen, and oxygen.



conversion processes, power system integration, electrochemical materials development, metabolic engineering of algae, and more. These advanced technologies are varied and complex, and each comes with its own set of challenges that must be addressed before they are ready for commercialization. It will take the creativity, hard work, and collaboration of scientists, engineers, and analysts from many disciplines throughout the Laboratory to meet these challenges and continue to move toward a sustainable hydrogen future.

hydrogenase enzyme, is responsible for releasing large amounts of hydrogen, even in the presence of limited photosynthetic oxygen evolution.

The process is reversible, and the cycle can be repeated over and over. To optimize hydrogen production, researchers are investigating cell density in the photobioreactors, the level of sulfate deprivation, the light intensity, the pH of the medium, and the presence of organic substrates in the medium.

Researchers are making steady progress in their endeavors to understand and direct the metabolic activity of *Chlamydomonas reinhardtii*, but photobiological hydrogen production is still an emerging technology with much to learn. Further investigation and optimization of both approaches will determine the most cost-effective, efficient route to hydrogen.

### Conclusion

The success of renewable hydrogen is directly tied to advances in renewable technologies under development at NREL — thermochemical

### Storing Hydrogen in Carbon Nanotubes

Developing safe, reliable, cost-effective ways to store hydrogen — with the ability to carry enough hydrogen on-board a vehicle to enable a 300-mile driving range — is critical to the success of the president's Hydrogen Initiative. But today's methods for storing hydrogen — under high pressure as a compressed gas, or as a liquid at extremely low (cryogenic) temperatures — cannot meet the performance requirements of on-board storage. Promising advanced solid-state materials like complex metal hydrides may provide a breakthrough in hydrogen storage. Another promising avenue, which NREL researchers are exploring, is nanostructured carbon materials that adsorb hydrogen gas reversibly at high efficiencies and energy densities.

### For More Information

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The basic mechanism that drives carbon-based hydrogen storage — gas-on-solid adsorption — is a safe, potentially low-cost method. However, high-surface-area carbon materials produced by conventional methods — pyrolysis of coal, biomass, or carbon carrying gases — do not adsorb significant amounts of hydrogen at room temperature. But carbon materials produced at the nanoscale (1 billionth of a meter) have dramatically different characteristics — large surface-to-volume ratios, unique size-specific chemistry, and short bulk diffusion lengths — that favor enhanced hydrogen adsorption.

To optimize the hydrogen adsorption capacity of carbon materials, we must understand the mechanism of the hydrogen adsorption, including the interplay between the chemical and molecular forces in bind-

ing hydrogen to carbon materials. Hydrogen can be adsorbed onto the carbon surface through physisorption, in which the physical attraction between molecular hydrogen and the carbon surface forms a weak physical bond, or through chemisorption, in which molecular hydrogen ( $H_2$ ) is dissociated into atomic hydrogen (H), forming a strong chemical bond with the carbon surface. To meet DOE's hydrogen storage requirements with this approach, the binding energy must permit strong but reversible immobilization of hydrogen atoms or molecules, and the density of the binding sites must be sufficient to ensure a system weight fraction of hydrogen of at least 8%.

During the past decade, NREL's R&D has focused primarily on the carbon nanostructure known as "single-wall nanotubes" (SWNTs), long, thin cylinders of graphite with a diameter of just a few hydrogen molecules (1-2 nm). The carbon atoms in the graphite structure are connected together in a hexagonal lattice similar to chicken wire. Researchers can control the synthetic conditions to produce tubes of different diameters, with different carbon bonding, and electronic type (semiconducting or metallic, a function of the nanotube lattice). They can also introduce defects, dopants, and catalysts into the nanotube structure to alter properties and tailor the performance of nanotubes.

In 1997, NREL researchers demonstrated that SWNTs can store hydrogen at a range they speculated to be 5%–10% by weight. More recently, they showed that SWNTs can adsorb up to 8% by weight hydrogen when catalytic metal species are present. However, other laboratories have not been able to duplicate these results. To resolve this controversy, NREL is now focused on improving the reproducibility of the measured performance and fully characterizing the SWNTs to understand the mechanism and extent of hydrogen adsorption.

Poor reproducibility is attributed in part to the small sample sizes currently available. Typically, NREL's SWNT samples weigh just a few milligrams. It is difficult to measure the performance of such small samples. NREL has established a group to define and disseminate measurement and sample-handling protocols for carbon nanomaterials. In addition, NREL scientists are developing repeatable and scalable methods for producing larger quantities of active materials.

They are also performing experimental and theoretical studies of carbon nanomaterials to uncover the fundamental science that drives the gas-on-solid adsorption process and to ultimately control and optimize hydrogen storage. As part of this endeavor, they are synthesizing, testing, characterizing, and evaluating a variety of different types of SWNTs and other carbon materials. They are investigating the impact of SWNT electronics and structure on the thermodynamics, kinetics, and capacity of

hydrogen storage, the role of defects and catalysts, and the nature of interactions at the SWNT wall/hydrogen interface. And they are exploring other nanostructured carbon materials, which could provide additional information on what governs adsorption interactions with hydrogen.

A number of new concepts have been proposed to explain and manipulate the hydrogen adsorption characteristics of carbon nanomaterials. One possible approach to increasing the hydrogen storage capacity of SWNTs is to enhance chemisorption with reversible hydrogen spillover. In this approach, a catalyst in contact with the nanotube wall dissociates molecular hydrogen. Because the nanotube is curved, the attractive forces of the carbon atoms in the lattice overlap. This results in a higher number of carbon atoms interacting with the hydrogen, which lowers the activation energy for hydrogen addition and permits surface diffusion of the hydrogen away from the catalyst. Atomic hydrogen diffuses from the catalyst onto the SWNT where it is stored. If the carbon-hydrogen binding energy is not too large, the process could be reversible.

Researchers still have a long way to go before this technology is fully understood. Significant improvements over currently available hydrogen storage technologies are required if hydrogen is to become a viable energy carrier. Innovative new approaches, improvements in synthesis and analysis techniques, and scale-up of optimized cost-effective processes are critical for determining the potential of these materials to store and release adequate amounts of hydrogen under practical operating conditions. Hydrogen storage represents a difficult but exciting challenge — success in unlocking the mysteries of hydrogen storage in nanoscale carbon materials could open the door to the hydrogen future.

One concept for increasing the ability of carbon single-wall nanotubes (blue) to store hydrogen is to use a metal catalyst (silver) in contact with the surface of the nanotube. Here, the catalyst dissociates hydrogen molecules to hydrogen atoms (yellow), which then diffuse into the nanotube lattice and reversibly bond with carbon atoms (blue).

# Unraveling the Structure of Plant Life

To Make Sustainable Fuels and Chemicals

Imagine the look on the bartender's face if you asked for your happy-hour cocktail to be 19 parts endoglucanase, 90 parts exoglucanase, and 1 part betaglucosidase. If you wanted a wood chips hors d'oeuvre, or to get energy from the fiber in your wheat crackers or corn chips, that enzyme cocktail would be just the thing. Endoglucanase, exoglucanase, and betaglucosidase are cellulases, a family of enzymes that act in concert to hydrolyze (decompose in water) the cellulosic fiber in plant material to sugar. The sugar can then be

used to make chemicals or ethanol fuel for our cars and trucks. According to NREL scientists, lowering the cost of the cellulases in that enzyme cocktail is the most promising avenue toward a competitive and domestic renewable alternative to gasoline. It is also a key element for developing a U.S. biorefinery industry that could make a wide range of chemicals and products from biomass — plants and organic wastes — as an alternative to chemicals derived from petroleum (see sidebar "What is a Biorefinery," page 12).

The United States already makes more than 2 billion gallons of ethanol per year from the starch in corn kernels and other grain. This is added as a 5% to 10% mixture to about one out of eight gallons of gasoline sold. But the primary use of corn is as animal feed, so it is relatively expensive, and there is a limit to how much ethanol can be made from it. NREL is developing technology to produce “cellulosic ethanol” from the fibrous material that makes up the bulk of plant matter. This dramatically increases the potential supply, adding inexpensive materials such as corn stalks and cobs, municipal wastes, sawdust and wood chips, and “energy crops” like grasses and fast-growing trees. Although the materials are relatively cheap, the conversion technology is not — yet. Currently, one of the biggest costs is for the cellulase enzymes used to convert cellulose to sugar. Although grain ethanol plants are sophisticated industrial operations, their underlying technology is relatively simple, similar to that used for moonshine stills. A common and inexpensive enzyme with a long history of industrial use for ethanol production — amylase — efficiently converts starch to sugar. Cellulases, however, are highly complex and do not have that history.

So NREL and DOE contracted with the world’s two largest enzyme companies, Genencor International and Novozymes — to reduce the cost of producing cellulases. The goal is to bring the cost of the enzymes down to about \$0.10/gallon of ethanol produced, which is key to making ethanol derived from cellulose economically competitive. Both companies are reporting excellent progress, but the goal is ambitious (see sidebar “Bringing in the Big Guns”) and the natural resistance of cellulose to decomposition makes the task challenging.

### The Recalcitrance of Biomass

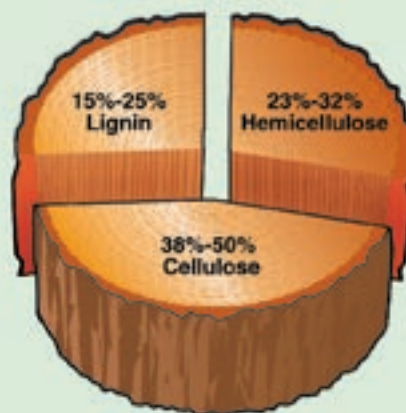
The name of the game is hydrolysis, breaking down complex carbohydrates (compounds of carbon, hydrogen, and oxygen) into their component sugars — analogous to how petroleum refineries break down complex hydrocarbons (compounds of carbon and hydrogen) into simpler chemicals, which are then built back up into desired fuels, plastics, and other chemicals.

The difference is that, unlike petroleum, plant carbohydrates are renewable. The vast bulk of plant material (most anything that is considered fibrous) consists of cellulose, hemicellulose, and lignin, with substantial starch and sugar found primarily in fruits and certain roots and tubers. Like starch and sugar, however, cellulose

and hemicellulose are carbohydrates. But the sugars of which they are made are linked together in long chains called polysaccharides, which form crystalline structures — nature’s plastics. Unraveling those polymeric structures is the key to economic biological conversion of cellulosic biomass to valuable fuels and chemicals. NREL scientist and cellulase expert Mike Himmel likes to refer to this complex and highly protective structure (the plant cell wall) as “nature’s cunning plan” to keep plants standing and resistant to microbes. He refers to the resulting challenge for bioconversion as the “recalcitrance of biomass.”

Cellulose consists of a loose crystalline structure of thousands of strands, with each strand containing hundreds of glucose sugar molecules (C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>). The cellulose is, in turn, wrapped in a sheath of hemicellulose and lignin, which further protects the cellulose. Hemicellulose is easier to hydrolyze than cellulose. A combination of heat, pressure, and acidic or basic conditions (each a way of causing hydrolysis, contributing an element of “severity”) breaks down hemicellulose into its component sugars. (Hemicellulose sugars are different from the glucose of cellulose and harder to ferment — but that’s another story). NREL researchers use dilute sulfuric acid for this thermochemical “pretreatment,” which hydrolyzes hemicellulose to its component sugars, making them soluble in water along with some of the lignin. The “solubilized” hemicellulose liquid can then be separated, leaving the cellulose and remaining lignin as solids. This pretreatment step not only hydrolyzes the hemicellulose, but also effectively removes the hemicellulose/lignin sheath from the cellulose, leaving the cellulose accessible to further hydrolysis.

Currently, cellulose is hydrolyzed in a similar fashion to the hydrolysis of hemicellulose, but with far greater severity, which is typically



So-called “cellulosic biomass” (trees, crop residues, municipal solid wastes, grasses, etc.) is primarily made up of cellulose, hemicellulose, and lignin. The proportion of these constituents varies with the type of biomass.

### Bringing in the Big Guns

To reduce the cost of cellulases, NREL and DOE contracted with the two largest enzyme companies in the world — Genencor International and Novozymes. Genencor sells enzymes and other biotechnology products for the health care, agri-processing, industrial, and consumer markets. Novozymes produces enzymes for a variety of markets and performs biotechnology research for the pharmaceutical, agricultural, and biochemical industries.

Both companies have already exceeded their initial objective, which was to reduce the cost of producing cellulases to one-tenth of what it was to start with. Having met their initial objective, they are performing follow-up work that could cut costs another several fold — to about \$0.10/gallon of ethanol produced. This will make enzymatic hydrolysis more cost-competitive and overcome a critical barrier for making cellulosic ethanol an economic reality along with grain ethanol. And, with the promise of the ongoing research to engineer even cheaper and more efficient cellulases, combined with advances in other aspects of biomass conversion technology, cellulosic ethanol may even become competitive with gasoline.

achieved with strong acid or higher temperature. This requires more expensive processing equipment — one reason why NREL researchers determined that biological (enzymatic) hydrolysis could be more cost-effective in the long run. (Another reason is that acid hydrolysis is fairly well developed, with little room for further cost saving, whereas enzymatic hydrolysis has great potential for cost reductions.) And cellulose can certainly be broken down biologically. Although humans cannot digest cellulose, cattle, termites, beaver, and mushrooms can. Some bacteria, fungi, and insects produce cellulases themselves; other animals host cellulase-producing bacteria in their digestive tracts. But, in keeping with the complex, recalcitrant structure of cellulose, even after the hemicellulose/lignin sheath is removed, enzymatic conversion is not simple.

### A Marvel of Nanomachinery

Most cellulases are systems of three types of enzymes, proteins that work together to catalyze biological conversion processes such as cellulose hydrolysis. First, an endoglucanase attacks one of the cellulose chains within the crystal structure, breaking it via hydrolysis, and creating new chain ends. During this hydrolysis, a molecule of water is consumed, and one of the chain ends becomes “reducing” and the other “non-reducing.” Then — in what is a remarkable example of nanoscale machinery — an exoglucanase attaches to a loose end, pulls the cellulose chain out of the crystal structure, and then works its way down the chain, breaking off cellobiose (dimers of two glucose molecules) as it goes. Actually, there are two types of exoglucanase to match the two types of loose chain ends. A cellobiohydrolase I (CBH I) attaches to the “reducing” end, and a cellobiohydrolase II (CBH II) attaches to the “non-reducing” end. Finally, a betaglucosidase splits cellobiose into two separate glucose molecules, making them available for processing into chemicals or fuels.

The dominant cellulase systems considered thus far for industrial processing have come from fungi, in particular from *Trichoderma reesei*. Cellulase researchers, however, also explore enzymes produced by other fungi and bacteria for traits or capabilities that might improve the enzymatic hydrolysis process. NREL scientists, for example, have investigated *Acidothermus cellulolyticus*, a bacterium they found in hot springs in Yellowstone National Park. Even though bacterial exoglucanases are not usually as good as fungal ones, they have a tolerance for high temperatures that could be used to speed up bioprocessing. The problem then becomes one of taking a fungus that normally grows on rotting wood scattered through the forest, mass producing it in a factory setting, extracting enzymes for industrial processing, and making the enzymes more effective by incorporating features such as the high-temperature tolerance of NREL’s hot springs bacterial enzymes.

### The High-Tech World of Protein Engineering

The two goals NREL set for Genencor and Novozymes (see sidebar “Bringing in the Big Guns,” page 11) are: (1) reduce the cost of producing the cellulases; and (2) make them more effective, so that less enzyme is needed. While the first avenue may include such mundane measures as optimizing growth conditions or processes, both lie predominantly in the high-tech world of protein engineering and production.

With genetic manipulation, you seek to turn genes on or off or to import genes that express a particular trait. In metabolic engineering, which NREL scientists practice to develop more effective fermentative organisms, researchers manipulate a series of different genes to give the organism the ability to digest a new food source or to produce more of a desired product such as ethanol. But NREL, Genencor, and Novozymes scientists are also going beyond these techniques. Instead, they are actually creating enzymes that never existed in nature and getting organisms to produce them.

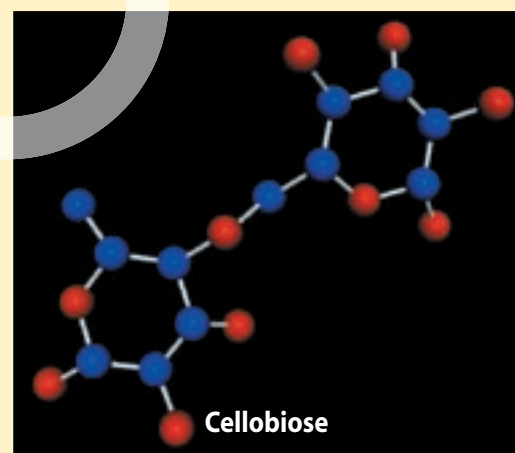
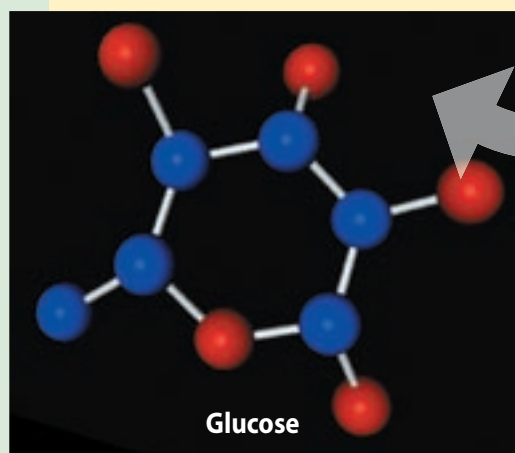
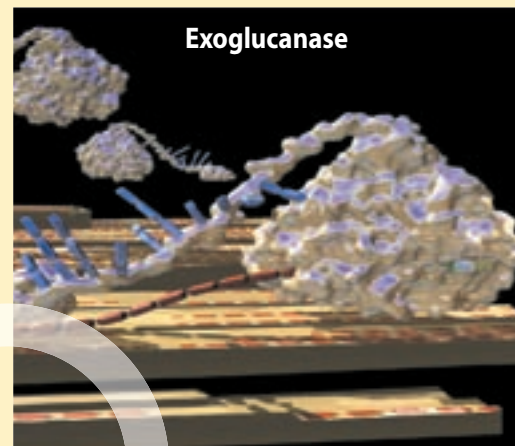
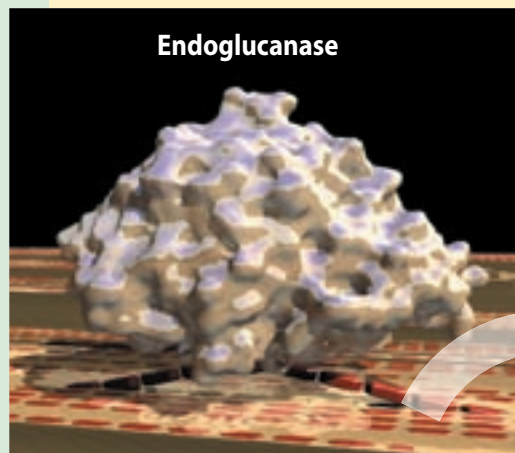
### What is a Biorefinery?

Once cellulase enzymes and bioprocessing technology are cost-effective enough to produce inexpensive sugar from cellulosic biomass, that sugar can become a “platform” chemical from which various fuels and chemicals can be made in “biorefineries.” The biorefinery concept is analogous to today’s petroleum refineries, which produce multiple fuels and products from petroleum. Industrial biorefineries have been identified as the most promising route to the creation of a new domestic biobased industry.

Wet-mill corn refineries now make ethanol, beverage sweeteners, and a variety of other food and animal feed products from cornstarch. Industrial giants Cargill-Dow (a joint venture between Dow Chemical and Cargill, Inc.) and DuPont are already making biomass plastics for clothing and other uses from lactic acid and 1,3 propanediol, both of which can be made from sugar or from cellulosic biomass. With lignin and hemicellulose sugars, as well as glucose from cellulose, the biorefinery will be even better positioned to make a variety of products.

The ability of an enzyme to catalyze a biochemical reaction is partly a function of the physical shape of the enzyme. In the illustration (right) of an exoglucanase — which Himmel refers to as “one of the most important proteins in the biosphere” — the “tadpole body” is the catalytic domain, and the “tail” is a binding site that “grabs onto” the cellulose and draws it into the body. The CBH I catalytic domain contains ten active subsites that physically adjoin to the cellulose and initiate the chemical reactions that break the chains apart into cellobiose. The question is, Can this nanomachine be improved?

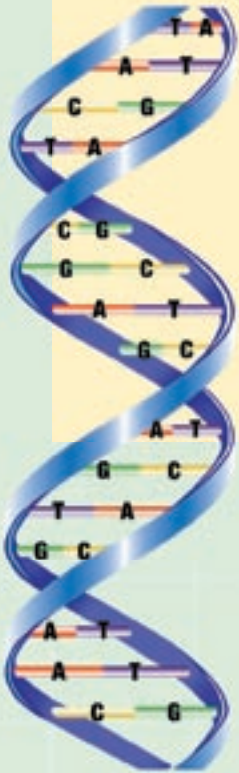
Assuming that improvement is possible, how do you get a fungi to produce a more efficient protein? To see how this may be done, it is necessary to understand how cells produce proteins. Ribonucleic acid (RNA) provides the code for producing proteins. But RNA itself is synthesized from a gene’s DNA (deoxyribonucleic acid), a polymer comprised of two strands of sequences of four nucleotides connected and wound around each other in a double helix configuration (see illustration, next page). The four nucleotides are guanine (G), cytosine (C), adenine (A), and thymine (T). Nucleotides on each strand attach to their complementary nucleotides on the other strand: G connects to C and A to T. To synthesize RNA, a polymerase enzyme attaches to a DNA and travels along the double helix.



**Cellulase enzymes break down cellulose to sugars in three steps. First, endoglucanase (top left) attacks a cellulose chain and severs it via hydrolysis; second, exoglucanase (top right) attaches to a cellulose chain end, works its way along the chain, and breaks off cellobiose molecules (bottom right); third, betaglucosidase splits the cellobiose into two glucose molecules.**

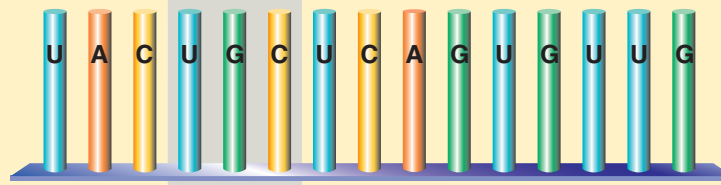
As it does so, it unzips the double helix into two strands, which zip back together as the polymerase passes along the DNA. One of the unzipped DNA strands serves as a template that the polymerase reads as it travels along, synthesizing a strand of RNA, whose sequence of nucleotides are the complements of the nucleotides read on the template. As the polymerase reads the sequence of nucleotides on the DNA template, it performs the trick of synthesizing a uracil (U) nucleotide for each adenine nucleotide it reads on the DNA (rather than producing the complementary thymine).

**By producing many products, biorefineries take advantage of differences in biomass components and intermediates and maximize value derived from biomass. For example, a biorefinery might produce several low-volume, high-value chemical products and a low-value, high-volume liquid fuel, while generating electricity and process heat for its own use and perhaps enough to sell electricity. High-value products enhance profitability. High-volume fuel helps meet national energy needs. Power production reduces costs and avoids greenhouse-gas emissions.**



## Protein Engineering

Codon for Amino Acid "Cysteine"



Sequenced triplets of RNA nucleotides, or codons, provide the code for a cell's ribosomes to manufacture chains of amino acids to make proteins. RNA itself is synthesized via copying the sequence of nucleotides of one of the strands of a gene's DNA. Hence, to engineer a protein, a first step is to devise a way to induce variations during the copying of a DNA's nucleotides.

Thus, the synthesized RNA is comprised of a sequence of A's, C's, G's, and U's — such as UGC UCA GUG; the sequence of which is divided into functional triplet nucleotides known as codons. Each codon codes for one of 20 amino acids. The codon UGC, for example, codes for the amino acid cysteine, while UCA codes for serine and GUG for valine. The codons on the RNA strand are read by the cell's ribosome machinery, which are "factories" that use the information provided by the codons to produce the amino acids. The string of amino acids thus produced is the primary structure of a protein. This primary structure then twists and folds to become a functional three-dimensional protein.

By manipulating the nucleotide sequence in the gene that codes for producing a particular cellulase in the fungi, scientists can change the sequence of amino acids in the cellulase, and thus alter its effectiveness — producing a designer protein. One way to change the nucleotide sequence is to use a bacterial polymerase that has been genetically engineered to incorrectly copy the genetic sequence to be modified. Or, scientists can subject a polymerase to abnormal conditions, such as high salt concentrations, which will induce the polymerase to produce variations when copying a DNA nucleotide. Using polymerases, researchers apply several techniques to engineer proteins, such as directed evolution and site-directed mutagenesis.

**Directed evolution.** In directed evolution, researchers randomly alter the nucleotide sequence of the particular fungal gene that codes for the exoglucanase or other protein produced. They then grow and test cultures of each of the altered fungi and select those with more desirable traits, such as greater enzyme production or enzymes with stronger hydrolysis activity. They tackle this Herculean task of seemingly infinite possibilities by using robotic equipment that can automatically culture

the possible genetic variants and screen them to identify the ones that exhibit the most desired characteristics. Researchers can then test the top candidates more thoroughly.

**Site-directed mutagenesis.** In contrast to the rapid-screening-of-random-changes approaches, with site-directed mutagenesis, researchers (1) build molecular models of the enzymes; (2) use computer simulations to examine the enzyme's structure and predict how it could be altered to more effectively interact with the cellulose strands; (3) identify the amino acid responsi-



NREL scientists use a robotics deck such as this to quickly culture genetic variants of fungal genes for producing enzymes and screen them to identify the variants with the most promising characteristics.

### What if Biomass Was Not So Recalcitrant?

The crystalline structure of cellulose and resulting fibrous nature of biomass may be one of nature's key features for protecting plant life in the biosphere — imagine a 200-foot-tall tree or even an 8-foot cornstalk otherwise — but that is not to say there are not other possibilities. NREL researcher Steve Thomas, who has worked on improving cellulases for breaking down cellulose, talks about starting

to look at the other side of the coin — altering the structure and composition of biomass. Thomas and colleagues are already examining many of the thousands of varieties of corn that seed companies have developed over the years to find ones that might be better for cellulose bioprocessing. Rather than just valuing high starch content in the kernels and tall and straight growth, cellulose bioprocessing could benefit from other traits. For example, corn plants with more cellulose in the stalk could benefit bioethanol



ble for the portion of the enzyme where change is desired; (4) identify the codon of nucleotides in the organism's genes that correspond to those amino acids in the enzyme, and; (5) set out to make the specific desired change in the DNA. At this point, they are back to inducing somewhat random changes. They know, however, that they have targeted the right site and more precisely what they are looking for in screening the variants.

### Modeling for Fundamental Understanding

Techniques such as site-directed mutagenesis require understanding the fundamentals of how cellulases function. One way to do this is through 3-D animation (see images of endoglucanase and exoglucanase, page 13), which can help researchers hypothesize how cellulases interact with cellulose. The hypotheses may then be tested to hone the picture. Another way is via modeling dynamic interactions, such as the surface layer interaction between water and cellulose, believed to be a key factor in the resistance of cellulose to hydrolysis and therefore in designing effective methods to overcome that recalcitrance. Modeling activities are invaluable in helping to understand the fundamentals of cellulase action. NREL researchers will continue to work in this vein, developing thermodynamic, mathematic, and mechanistic models of the molecular machinery of enzymatic hydrolysis.

### Moving to Eureka! and a Biomass Economy

Just as understanding basic science behind cellulase activity is critical for specific applications such as site-directed mutagenesis, it is also where dramatic changes in approach could come from. Himmel expects the "Voila!s" and "Eureka!s" of enzymatic hydrolysis to come from fully understanding the way the exoglucanases work. Industry does not generally do such basic research, so DOE has asked NREL to lead in this area. NREL's work to gain understanding of this crucial research area is supported by collaborations with Cornell University, the Colorado School of Mines, the University of California at Davis, Rutgers University, the University of Arkansas, and research institutes in Japan, Israel, and Sweden.

On the other hand, NREL cannot begin to develop the real-world improvements associated with actual industrial operations that can come from enzyme producers such as Genencor and Novozymes. NREL researchers are validating the achievements of the enzyme companies. And, of course, research understanding will do no good unless industry incorporates it into practice. So, overcoming the recalcitrance of biomass with economical enzyme production — which will lead to more cost-effective production of ethanol and other products from cellulosic biomass — must come from a combination of basic research at NREL and universities and from steady improvement by the enzyme industry.



One way in which researchers gain insight into how cellulases function is through the development and use of models, such as this one of the dynamic interaction at the interface between water and cellulose.

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production, or ones with more lignin could benefit biomass power generation. Using NREL's rapid analysis technology for biomass and sophisticated economic models, researchers have already found that ethanol production could be more than \$0.30/gallon less expensive using stover with different composition.

Going a step further, many plants produce enzymes that break down their own cell walls, with the enzymes serving

functions such as ripening fruit or allowing leaves to break off in the fall. We could breed plants with high natural cellulase production, genetically engineer higher or earlier production of the cellulases, or import cellulase production genes from fungi. One possibility is plants that already start to break themselves down before they are harvested. Another possibility could be one part of a plant producing enzymes needed to break down other parts. Either would make the work of the biorefinery easier and less costly.



# Winds of Change

## Offsetting CO<sub>2</sub> Emissions with Wind Energy

“Climate change is occurring,” says John H. Marburger III, director of the White House Office of Science and Technology Policy. The Intergovernmental Panel on Climate Change (IPCC), a group of 2900 leading climate scientists from 120 countries, agrees. Climate change could lead to rising sea levels, ecological instability, and a growing incidence of weather anomalies such as floods and droughts — changes that are likely to have consequences for the world environment and economy.

IPCC scientists agree that climate change is the result of growing emissions of carbon dioxide (CO<sub>2</sub>) and other greenhouse gases from anthropogenic (human) activities — deforestation, industrial processes, and fossil fuel combustion. As these gases accumulate in the atmosphere, they trap heat, creating a greenhouse effect.

Roughly 84% of the anthropogenic contribution to climate change is due to CO<sub>2</sub>; the rest comes from gases such as methane, which traps 23 times more heat per gram of gas than CO<sub>2</sub>, and nitrous oxide, which traps 296 times more heat. Even if all anthropogenic emissions were to stop tomorrow, the concentration of greenhouse gases in the atmosphere would take centuries to return to preindustrial levels. The IPCC has estimated that, to maintain stable atmospheric conditions in the long run, anthropogenic emissions of greenhouse gases must be cut 60% to 70%.

The United States itself produces about 23% of global greenhouse gas emissions. Plus, with a growing economy, U.S. emissions continue to increase at a rate of about 1% per year.

## The Energy Connection

Most U.S. greenhouse gas emissions come from our reliance on fossil fuels, which are made up primarily of hydrogen and carbon. When burned, the carbon combines with oxygen to yield CO<sub>2</sub>. In 2002, electricity production was responsible for 2249 Tg (teragrams, or million metric tons) of CO<sub>2</sub> emissions, or 39% of the U.S. total.

The U.S. government is considering ways to mitigate the problem, including voluntary measures to decrease U.S. greenhouse gas intensity — the ratio of emissions to economic output — by 18% during the next decade. In February 2003, speaking about the need to curb emissions, Energy Secretary Spencer Abraham said “We will also need to develop the revolutionary technologies to make these reductions happen. That means creating the kinds of technologies that . . . actually transform the way we produce and consume energy.”

Wind energy is such a breakthrough technology. Because wind power plants produce virtually no CO<sub>2</sub> emissions during operation, grid-connected wind power reduces overall greenhouse gas emissions by displacing the need for natural gas- and coal-fired generation.

## The Wind Resource

Wind power is among the world’s fastest-growing sources of energy. In 2003, U.S.-installed wind generation grew by 1687 MW (greater than 30%) to 6374 MW. Worldwide, more than 8000 MW of wind capacity was added, bringing the international total to 39,000 MW.

The United States has enough wind resources to meet more than twice the nation’s total electricity demand. Wind resources are characterized by wind-power density classes, ranging from Class 1 (lowest) to Class 7 (highest). Fair to good wind resources (Class 3 and above), which have an average wind speed of at least 13 mph at a 50-m hub height, are found along the East Coast, the Appalachian Mountains, the Great Plains, the Pacific Northwest, and other areas. North Dakota alone has enough Class 4 and higher winds to supply a third of the electricity needs of the lower 48 states.

## Using Wind Energy to Cut Emissions

Although a wind plant produces no CO<sub>2</sub> while generating electricity from wind, it does take fossil energy to mine, transport, and fabricate materials used in plant construction; build the power plant; operate and maintain the plant during its

service life; and decommission the plant at the end of its useful life.

According to a 1989 DOE study, when all energy requirements are taken into account, a wind plant adds about 7.4 g of CO<sub>2</sub> to the atmosphere per kilowatt-hour of electricity generated. But this is lower than 964 g/kWh for a typical coal-fired plant, 484 g/kWh for a natural gas turbine plant, and 611.7 g/kWh generated by the average U.S. utility mix (which takes into account the electricity generated by a weighted mix of hydropower, nuclear power, coal, natural gas, and other generating technologies). Wind power thus can displace 956.6 g/kWh of CO<sub>2</sub> from coal plants, 476.6 g/kWh from natural gas plants, and 604.3 g/kWh of CO<sub>2</sub> from the average U.S. supply mix.

According to estimates by the DOE’s Energy Information Administration (EIA), total electricity demand will increase from 3839 billion kWh in 2002 to an estimated 5430 billion kWh in 2020. The great majority of this increase is expected to come from the use of new natural gas and coal-fired plants. A good portion of this increase is also expected to come from wind turbines. In fact, members of the wind energy industry project that wind-generated power will provide 6% or more of the nation’s electricity by 2020 (roughly 326 billion kWh). This would entail an average yearly growth rate of approximately 18%.

On the other hand, if the wind market grew at an annual rate of 28% (a growth rate that is less than that for the world market during the past five years), then in 2020 wind energy would provide approximately 20% of the nation’s electricity — which is often considered to be the maximum amount of wind energy that can be incorporated into the electricity grid without adversely affecting grid reliability (see also discussion on page 20). If wind has a 20% share of the electricity market in 2020, wind power plants will be generating about 1086 billion kWh; this would require roughly 413 GW of installed wind capacity, assuming an average capacity factor of 30% (see sidebar “Calculating Energy Output from Wind Turbines”).

## Calculating Energy Output from Wind Turbines

Wind turbines are usually classified according to their rated electric power output, e.g., 1 MW. This means the turbine can produce a maximum of 1 MW of power in ideal wind conditions. But because wind is an intermittent resource, the wind turbine won’t be operating at its maximum rated capacity all of the time. The average capacity at which the turbine operates during the course of its lifetime is called its capacity factor.

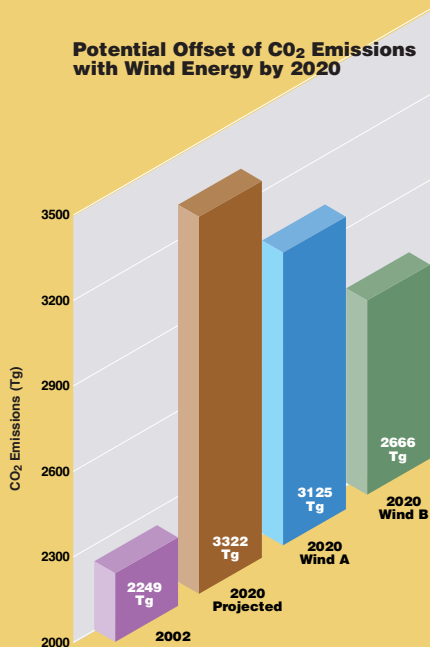
The question is how much electric energy (electricity) a wind turbine of a rated power output could produce over time. Energy production is usually determined by the equation: Energy = Power x Time. For electricity generating plants, this can be more accurately be restated as: Energy = Power x Time x Capacity Factor, where the capacity factor is the ratio of the amount of energy produced over time to the amount of energy that could have been produced if the turbine operated at its maximum rated output 100% of the time.

For example, with a capacity factor of 30% and 8760 hours in a year, the energy produced by a 1-MW wind turbine over the course of a year would be: 8760 h x 0.30 x 1 MW = 2628 MWh.

A turbine’s capacity factor is affected by the amount of down time required to service the turbine and by the site-specific wind conditions. The more time the turbine spends in service, and the lower the average wind speed at the site, the less energy the turbine produces, hence the lower the turbine’s capacity factor.

Capacity factors can vary widely. Today’s nationwide fleet of wind turbines is operating at an average capacity factor of 30%, and this ratio is improving. The American Wind Energy Association (AWEA) estimates that turbines installed since 2001 are operating at an average capacity factor of about 33%, and EIA estimates that, by 2020, some new turbines will be operating with capacity factors of 42% to 48%.

### Potential Offset of CO<sub>2</sub> Emissions with Wind Energy by 2020



The EIA projects that CO<sub>2</sub> emissions from power plants could increase to 3322 Tg by 2020. But if wind energy supplied between 6% and 20% of the nation's electricity by then, the expected rise in CO<sub>2</sub> emissions would be reduced by 197 Tg (Wind A) to 656 Tg (Wind B), assuming that the wind energy would displace the average utility generation mix.

Using today's electricity supply mix and emission rates, CO<sub>2</sub> emissions from the electricity sector in 2020 would be about 3322 Tg, an increase of 1073 Tg. On the other hand, if wind energy could supply between 6% and 20% of the nation's electricity, wind would reduce the expected CO<sub>2</sub> emissions by between 197 Tg and 656 Tg — a significant impact under either scenario.

### Getting There

A 6% market penetration of wind energy by 2020 not only appears to be an attainable growth scenario, but this amount of wind energy could easily be incorporated into the electricity grid despite an intermittent wind resource.

But how realistic is it to think that wind could provide 20% of the nation's electricity by 2020? In terms of achievable market growth, 20% is optimistic. In terms of resource, it could be accomplished without much difficulty — according to DOE, to provide 20% of America's electricity from wind, only 0.6% of the land of the lower 48 states would have to be developed with wind power plants. Much of the land could be used for a dual purpose — for both farming and wind energy, providing farms with an extra "cash crop."

What about intermittency? At deployment levels up to about 20%, wind power can be incorporated into the electricity grid relatively easily. The U.S. power grid already includes generating assets, such as hydroelectric power, that can be used to compensate for wind's intermittency. And wind forecasting software can overcome many of the challenges associated with intermittency.

What about intermittency? At deployment levels up to about 20%, wind power can be incorporated into the electricity grid relatively easily. The U.S. power grid already includes generating assets, such as hydroelectric power, that can be used to compensate for wind's intermittency. And wind forecasting software can overcome many of the challenges associated with intermittency.

According to Britta Buchholz of MVV Energie, German wind forecasters are currently able to predict wind strength and power output 48 hours ahead with 90% accuracy. As wind conditions can vary significantly from one place to another, the geographical disbursement of turbine arrays tends to decrease the variance in wind power output. This is because a drop in output from one wind farm can be made up by a rise from another.

Denmark, which gets about 17% of its electricity from wind, is starting to have some problems integrating wind power into its electricity grid. This is because Denmark is a small country that doesn't have enough geographical variability in wind patterns to even out fluctuations in wind strength (and hence turbine output). Small wind projects of single turbines or small clusters of turbines contribute the majority of Denmark's wind power.

If wind-generated electricity grows to comprise more than about 20% of power flows on the grid, the intermittency of the wind resource could pose a problem for grid system operators. Some form of backup generation (such as natural gas) or of energy storage would have to be used to compensate for wind's intermittency. Although exact data are not available, it is clear that this would degrade the energy payback ratio somewhat and would slightly increase emissions of CO<sub>2</sub>. It is also likely that upgrades to the transmission infrastructure would be required for wind energy to service major load centers, although the cost of these improvements may not be prohibitive. NREL has estimated that 175 GW of wind capacity lie within 5 miles of existing 230 kV or lower transmission lines, and another 284 GW lie within 10 miles. In a series of letters to *Science* magazine in fall 2001, Stanford University researchers Mark Jacobson and Gilbert Masters concluded that, even assuming a relatively high average cost of \$500,000 per mile to build new above-ground AC transmission lines, the cost of the new lines would add less than 1% to the cost of the wind

### Reducing the Cost of Wind Energy

NREL is home to DOE's National Wind Technology Center (NWTC), where the main focus is to work with the wind industry to improve wind energy technology and decrease its cost. NWTC researchers are working with industry to develop new breeds of wind turbines that will operate efficiently in Class 3 and 4 wind regimes, with the goal to reduce costs for Class 4 areas to 3¢/kWh on land and 5¢/kWh offshore by 2012, and to reduce the cost of wind energy in Class 3 regimes to as little as 10¢/kWh by 2007.

One strategy for exploiting lower-class wind regimes is to develop advanced large turbines (1 MW or greater). Because they have a

higher hub height where the wind typically blows stronger, and because larger blades are used to sweep greater areas, large turbines can harvest more energy for a given wind class. For these advanced concepts, researchers are considering every component — from the base of the tower to the tips of the blades — for opportunities to improve the technology.

They are, for example, researching blade sizes and shapes, and better and lighter materials with which to make blades and towers that last longer, extract more energy, and cost less to manufacture. They are investigating alternative concepts for drivetrain components (gearboxes, generators, and associated power electronics) that

## Calculating the Energy Payback from Wind Turbines

Power plants consume energy even before they begin making it. Materials to be used in the plant must be mined, shipped, and fabricated; power plant parts must be transported to the construction site and assembled; the plant must be operated and maintained; and the plant must be disassembled and decommissioned at the end of its service life.

The time it takes for a power plant to generate as much energy as it uses over the course of its life is called the energy payback time. The energy payback of a power plant can also be expressed as the ratio of the energy generated by a power plant during its lifetime to

the energy required to build, operate, and decommission the power plant.

According to European studies, a typical utility-scale wind turbine will produce, on average, 30 times more energy than it consumes during its lifetime. According to AWEA, a wind turbine's energy payback period is typically three to eight months, depending on the average wind speed at the site. Moreover, because energy payback is typically a measure of how long it takes to pay back fossil fuel energy, it is also a measure of how long it takes to pay back the CO<sub>2</sub> emitted by the consumption of that fossil fuel. In contrast, because they must consume fossil energy to produce electricity, fossil fuel power plants never achieve energy, or CO<sub>2</sub>, payback.

power plants. (Note that their analysis assumes that existing transmission lines have room to carry the wind-generated power.)

### What about the affordability of wind power?

According to DOE, new, utility-scale wind projects are being built in the United States today with energy costs ranging from about 3.9¢ to 7¢/kWh or more. The lower-cost wind energy is typically achieved for the better wind sites, such as Class 6. Wind energy at Class 4 sites, on the other hand, is currently marketed at prices in the 5¢ to 7¢/kWh range. In comparison, DOE's National Energy Technology Laboratory (NETL) reports that the average cost of electricity from current coal-generating facilities is 4¢/kWh and about 3.5¢/kWh from state-of-the-art facilities. NETL also projects that the cost of electricity from advanced coal facilities could be reduced to 3.1¢/kWh by 2010.

With the cost of wind power in the better wind regimes close to that of coal power, expanding the proportion of wind-generated electricity in the energy supply mix is not expected to have much of an impact on future electricity prices. A 2002 EIA study concluded that a federal renewables portfolio standard (RPS) requiring 10% of electricity to be generated from renewable sources by 2020 would result in a 1% increase in retail electricity prices, while a 20% RPS would result in a 3% increase. The study predicts that most new renewable electricity would come from wind, despite the fact that it assumes there will be no federal production tax credit for generation from wind plants and no renewable energy production incentive.

As researchers at NREL and in industry lower the costs even more, especially for wind turbines operating in Class 3 and 4 wind regimes, wind could become highly competitive with all other sources, and may even become the power of choice for many areas of the United States. If such becomes the case, wind energy could grow sufficiently to supply the United States with 20% of its electricity and could help the nation and the world find the means to decrease greenhouse gas emissions while meeting the energy needs of a growing economy. (See sidebar on "Reducing the Cost of Wind Energy.")

### For More Information

American Wind Energy Association. (2002). "The Most Frequently Asked Questions About Wind Energy." <http://www.awea.org/pubs/documents/FAQ2002%20-%20web.PDF>. Accessed Jan. 29, 2004.

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could result in less weight and more efficiency. And they are exploring new rotor designs to extract more energy from the wind and to reduce peak and fatigue loads.

NWTC researchers are also performing field and air-tunnel tests. They are using the results from the tests to develop computer simulations and models that will:

- enable them to accurately project how wind turbines react to varying wind conditions;
- help them better forecast wind conditions and understand the characteristics and location of wind resources so that developers can site wind farms in the best locations; and

- allow them to predict the performance of advanced prototype designs, reducing development time and costs.

The NWTC also provides world-class testing facilities. At the structural test facility, researchers can determine strength and durability of full-scale wind turbine blades. At the dynamometer facility researchers test the lifetime endurance of a wide range of wind turbine drivetrains and gearboxes at various speeds. Results from both facilities help turbine designers increase the lifetimes of blades and components by decreasing loads on the components, or making them more efficient and resistant to wear — thus increasing the life and reliability of wind turbine components and reducing costs.

# Awards & Honors

Since the last publication of the *Research Review*, NREL, its researchers, and partners have received several awards and honors. Among these are four R&D 100 awards, two tech transfer awards from the Federal Laboratory Consortium (FLC), recognition by *Scientific American*, and a newly elected fellow of the American Association for the Advancement of Science (AAAS).

## PPS Protection

Carbon steel is tough, but not tough enough to withstand harsh conditions found in geothermal power plants, chemical plants, and railroad tank cars.

To protect vital fluid-carrying steel tubes in hostile environments, re-

ment and commercialization. Within nine months of first being contacted about the technology by NREL and BNL, the company had incorporated PPS into a commercial product. It now repre-

sents the primary line of business for Bob Curran & Sons, which has built a new facility near Houston to better serve its burgeoning roll of customers in the petrochemical processing industry.

A PPS coating is not only tough, it is smart. Its three-layer construction divides the duties, with the innermost one — a zinc phosphate ceramic primer — assigned to create a strong bond with the steel. The second layer, typically a carbon fiber PPS matrix, provides toughness, corrosion protection, and high thermal conductivity. The third layer, a polymer blend of PPS, calcium bialuminate, and Teflon, gives the product a self-healing mechanism that repairs damage to the coating system by filling in small cracks due to physical wear.

PPS extends the life of untreated carbon steel by fivefold. Even when compared to stainless steel or titanium tubes, PPS-coated carbon steel tubes yield a life-cycle cost savings of up to 82%.

## Nanofiber Protection

New alumina ceramic nanofibers developed by NREL, Argonide Corporation, and the Design Technology Center of the Russian Academy of Sciences can be used in bioactive filtration to eliminate 99.99999% of a variety of viruses, bacteria, and pathogens from fluids. This includes hepatitis A, retroviruses, adenoviruses, coxsacke, Salmonella, shigella dysenteriae, and E. Coli. The fibers also can be used in bone tissue engineering, to eliminate 99.99% of heavy metals in water, and to reduce arsenic in drinking water to well below federal and international standards.

The fibers' remarkable capabilities derive from their unique combination of small diameter (about 2 nm), long length (up to hundreds of nm), a surface area of 600 m<sup>2</sup>/gm, and surface chemistry that can be tailored. Trademarked and marketed as NanoCer-am by the Argonide Corporation, the nanofibers arrive with good timing, in light of heightened concerns about bio-terrorism and national security.

## Letting in Light

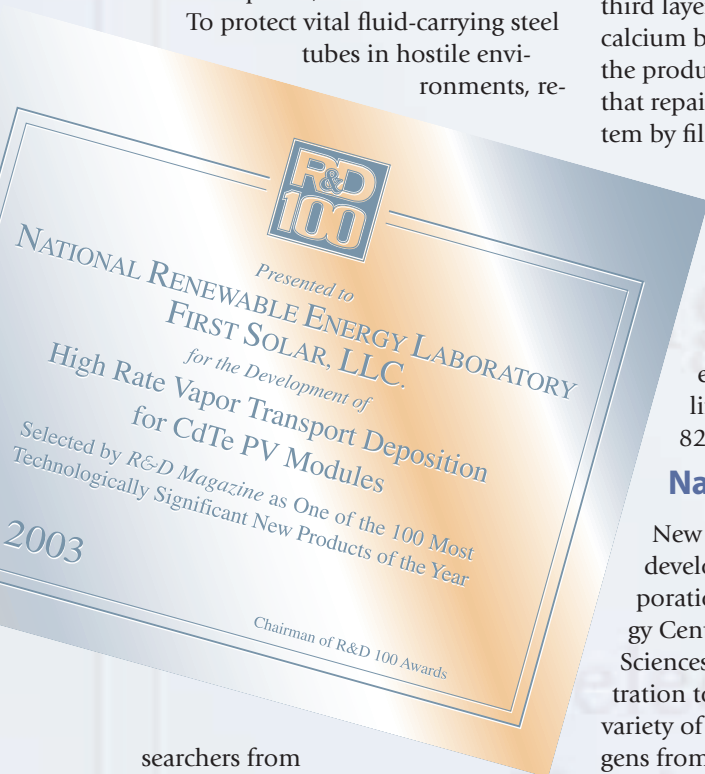
BP Solar's PowerView module, developed jointly with NREL, doubles as architectural glass and a PV module. Particularly useful for sloped glazings such as awnings, BP has installed it at hundreds of its Connect fueling and retail sites, where much of the electricity demand is met with their own futuristic, semi-transparent canopies.

Helping make PowerView possible was an innovative manufacturing method from BP Solar, in which programmable lasers were used to selectively remove material from the thin-film PV module to allow light through while minimizing the decrease in electrical power. Although an innovative technology, this R&D 100-award winner fell victim to a BP Solar reorganization that dropped thin-film modules from the company's PV product line.

## A Module a Minute

First Solar's automated, non-stop, continuous-feed production line can crank out one PV module per minute — and these are 60 cm x 120 cm, high-quality modules made of thin-film cadmium telluride (CdTe) and cadmium sulfide (CdS). How is it done? Soda-lime glass is fed into vacuum deposition chambers where a layer of CdTe is deposited on the glass, followed by a layer of CdS. The modules are then laser-scribed, metallized, and encapsulated in ethyl-vinyl acetate, and then another layer of soda-lime glass.

The enabling core of this process is the R&D-100-award-winning high-rate vapor transport deposition technology developed by First Solar and NREL. This is a deceptively simple technology that can deposit a thin, uniform



searchers from NREL and Brookhaven National Laboratory (BNL) developed a polymer-based coating system called polyphenylenesulfide (PPS). This technology, which won both an R&D 100 award and an FLC technology transfer award, was transferred to Bob Curran & Sons for further refine-



**Dr. Bhushan Sopori demonstrates PVSCAN, one of the technologies that he developed and helped transfer to industry, and for which he won an FLC award.**

layer of CdTe or CdS on glass substrate in less than 40 seconds — a deposition rate three to four orders of magnitude greater than rival thin-film PV technologies.

It is the world's first such mass-production method for making polycrystalline thin-film modules. In its first year of production, the technology helped First Solar cut the price of PV modules to \$2.50 per watt. A second-generation production line now under construction could lower the price by nearly another 50% in the next three years.

### Monitoring Manufacturing

By transferring two related technologies to GT Equipment Technologies, Inc. (GTi), a manufacturer of equipment for semiconductor and PV materials processing, NREL helped fill a need in the international solar energy community.

One of the two technologies, PVSCAN, is a high-speed, optical-scanning system that maps and analyzes defects in PV wafers and cells. The other, the PV Reflectometer (marketed as the GT-Fabscan 6000), is used to monitor important parameters in solar-cell processes including surface roughness and texture, metallization, antireflection coatings, and back contact properties.

The theory behind both technologies, as well as their design and engineering, are products entirely of NREL researchers, who also helped negotiate licensing of the technologies by GTi and worked closely with the company

to scale them up to production. These efforts will yield additional benefits to NREL in the form of new relationships with R&D groups, universities, and PV makers and other companies from the United States and abroad.

### Scientific American 50

In its debut issue of spotlighting the top 50 business and research leaders of the year, *Scientific American* magazine recognized NREL and Spectrolab, Inc. as leaders in the energy category for their work in increasing the efficiency of PV cells.

NREL's research in multijunction solar cells for more than a decade has led the way to ever-more-efficient cells, offering the potential of cheaper electricity from the sun. Multijunction solar cells use multiple layers of semiconducting material to absorb sunlight and convert it to electricity more efficiently than single-junction cells.

In 2001 — using a solar-cell design licensed from NREL — Spectrolab made a gallium indium phosphide/gallium arsenide/germanium (GaInP<sub>2</sub>/GaAs/Ge) triple-junction solar cell that converted 34% of sunlight to electricity under concentration — a world record at the time. Since then, the company has improved the conversion efficiency to 36.9% under 309 suns concentration.

This technology has won two R&D 100 awards. The first was won by NREL in 1991 for a double-junction cell (GaInP<sub>2</sub>/GaAs) whose primary use

is for space applications. The second award was presented to both NREL and Spectrolab in 2001 for the triple-junction device.

### Art Nozik Elected AAAS Fellow

Arthur J. Nozik was recently elected a fellow of the American Association for the Advancement of Science, the highest distinction bestowed on AAAS members by their peers

Dr. Nozik is a senior research fellow at NREL. During his tenure at the Laboratory, he has established himself as a leader in photoelectrochemistry, semiconductor-molecular interfaces, quantization effects, carrier dynamics, and the application of these interdisciplinary sciences to the conversion of photon energy to electricity or fuels (such as hydrogen or alcohols).

Dr. Nozik received his Ph.D. in physical chemistry from Yale University in 1967 and joined NREL in 1978, where he has been a research fellow since 1983 and has been recognized with several important Laboratory-wide distinctions, including the Van Morris award, the Hubbard Award, and an award for outstanding achievement. He has published more than 160 peer-reviewed publications, edited several books in his fields of expertise, been awarded 11 U.S. patents, and served as a senior editor on *The Journal of Physical Chemistry* since 1993.



**Dr. Arthur Nozik becomes a fellow of the AAAS.**

# NREL in Focus

## First Director Joins National Bioenergy Center

DOE's National Bioenergy Center, based at NREL, welcomed Dr. Michael Pacheco as its first director in 2003. Pacheco arrived with an impressive resume from private industry, most recently with Louisiana-Pacific Corp., for which he was manager of oriented strand board technology and product quality. He also spent two years as a corporate engineering fellow with the company.

Pacheco has led efforts to commercialize biocatalytic processes with Texas-based Energy BioSystems Corp., where he was vice president of process development. He held numerous supervisory R&D positions during 13 years with Amoco Corp. and three years with Conoco Oil Co. Pacheco holds a Ph.D. in chemical engineering from the University of California at Berkeley, a bachelor of science in chemical engineering from Clarkson University, and an associate degree in chemical technology from Thames Valley College.

Pacheco will provide strategic guidance, technical direction, and management to continue the center's leadership role in bioenergy research. His responsibilities include coordinating NREL's activities with bioenergy research at Argonne National Laboratory, Idaho National Energy and Environmental Laboratory, Oak Ridge National Laboratory, and Pacific Northwest



**Dr. Michael Pacheco becomes director of the National Bioenergy Center.**

The Bioenergy Center was created in 2000 as the focal point for developing bioenergy technology and information in the United States. It gives industry "one-stop shopping" for world-class

research and state-of-the-art laboratory facilities at several federal agencies. As the center's new director, Pacheco replaces acting director, Stan Bull, who is NREL's Associate Director for Science and Technology.

The center links DOE-funded biomass renewable energy research programs with the resources and capabilities of the U.S. departments of Agriculture and Interior, the Environmental Protection Agency, the National Science Foundation and several other federal agencies, DOE laboratories, universities, and the private sector. NREL's biomass research program focuses on converting biomass feedstocks into transportation fuels, chemicals, biobased materials, and electric power.

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## Seibert Named Research Fellow

In October of 2003, internationally recognized research scientist Michael Seibert was named

National Laboratory. Pacheco will represent the interests of DOE, NREL, and the other labs to technical and industrial leaders and to various U.S. and international stakeholders.

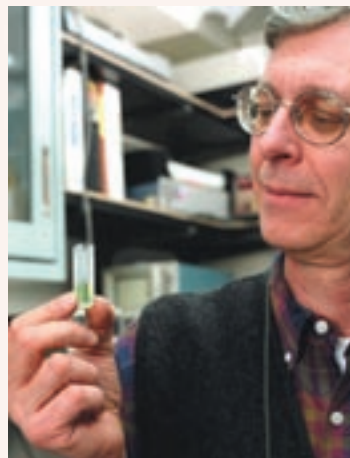
as the newest member of NREL's Research Fellows Council. An NREL employee since 1977, Seibert has devoted his career to researching structure and function problems in photosynthetic energy capture, biological water-splitting processes, and photoproduction of hydrogen by algae.

Before becoming an NREL research fellow, Seibert was elected a fellow of the American Association for the Advancement of Science. He currently serves on the editorial boards of *Advances in Solar Energy*, *Applied Biochemistry and Biotechnology*, and the *American Institute of Physics International Series in Basic and Applied Biological Physics*. Seibert has established scientific and technical collaborations throughout the world; authored more than 170 scientific articles and reviews; and given more than 150 conference presentations. He holds eight U.S. and foreign patents.

Seibert holds a Ph.D. in molecular biology and biophysics, and an M.S. in physics, both from the University of Pennsylvania; and a B.S. in physics from Pennsylvania State University. He was born in Lima, Peru and grew up near Philadelphia.

The Research Fellow and Senior Research Fellow positions at NREL were established to provide parallel or dual career opportunities for outstanding scientists and engineers who have achieved exceptional positions of leadership in their fields, but who wish to

devote the majority of their time and energy to scientific and technological endeavors. Candidates are nominated by senior management and current research fellows. Seibert joins Art Nozik, Alex Zunger, Tim Coutts, Dick Ahrenkiel, and Ralph Overend on the NREL Research Fellows Council.



**Dr. Michael Seibert is named to NREL's Research Fellows Council.**



## S&TF Plans Move Ahead

NREL's much-needed Science and Technology Facility (S&TF) took a big step closer to becoming reality in November 2003, with \$4 million in funding for its first phase of construction approved in the Energy and Water Development Appropriations Act of 2004. Construction is expected to begin in the late summer of 2004 and be completed in approximately two years.

Construction of the proposed semiconductor research facility is estimated to cost a total of \$20.2 million. It will be located 80 feet to the east of the existing Solar Energy Research Facility (SERF) and will include 71,000 square feet of laboratory, office, and support space on three levels. The building will be connected to the SERF via an elevated bridge that links the service corridors of the two buildings, thereby facilitating collaboration between researchers in the two facilities. Approximately 75 research staff will work in the new facility.

The facility-design process — completed on time and within budget — was no small feat, says Pete Sheldon, a division manager who represented

the National Center for Photovoltaics in designing the facility. The process solicited input from an NREL team of experienced researchers, chosen to ensure that current and future research requirements will be met. The team also included representatives with expertise in energy-efficient building design, daylighting, sustainability, and environmental health and safety.

Research capabilities within the new S&TF, combined with those of the existing SERF, will enable new and expanded work in photovoltaics, hydrogen, solid-state lighting, electrochromic windows, and basic sciences, including nanotechnologies.

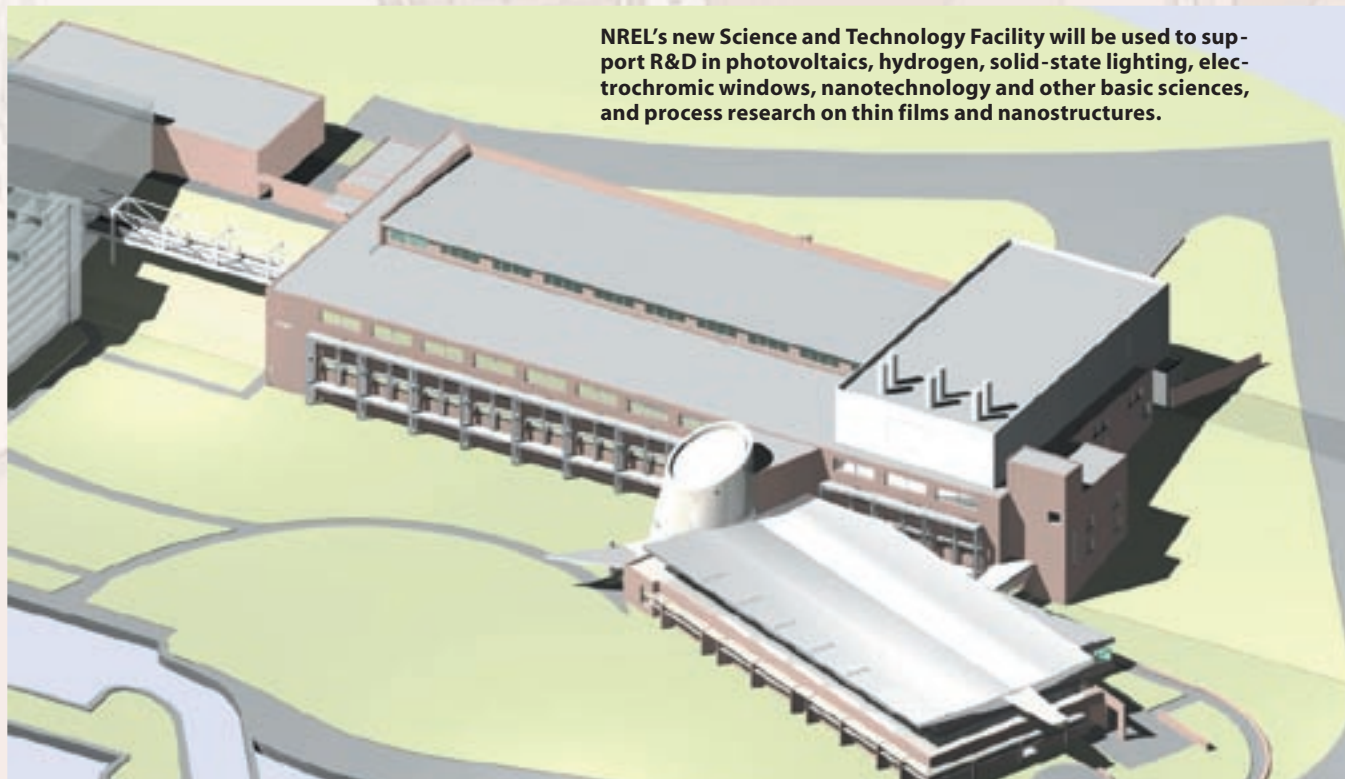
The S&TF will support process research on thin films and nanostructures for DOE and for U.S. companies developing energy technologies. It is designed around a process research concept specifically developed to accelerate the time required to transfer research developed in the laboratory to manufacturing and use, Sheldon says. The centerpiece of the building is the Process Development and Integration Laboratory — an open 11,000-square-foot lab space specifically designed to accommodate a new class of thin-film depo-

sition, processing, and characterization tools. These tools will provide new ways to bridge the gap between laboratory and commercial success, by allowing researchers to flexibly prototype processes in a controlled environment.

The facility was designed with sustainability in mind. The multi-story design reduces the building footprint to approximately 45,000 square feet, thereby conserving valuable land for future expansion opportunities. It exploits a state-of-the-art energy efficient mechanical design that reduces energy use by 50%, compared with a DOE 10CFR434 compliant building. And it will provide 100% of the ambient light requirements in the open office and circulation areas, while maximizing daylighting opportunities in the laboratories.

## Lab Takes on Hydrogen Systems Integration

With the nation's high expectations for hydrogen as an important energy carrier comes a new, high-profile responsibility for NREL. The Laboratory was designated the central systems integrator for DOE's hydrogen efforts as of March 2003.



**NREL's new Science and Technology Facility will be used to support R&D in photovoltaics, hydrogen, solid-state lighting, electrochromic windows, nanotechnology and other basic sciences, and process research on thin films and nanostructures.**

The role includes documenting technical requirements of a future hydrogen energy system for the United States, and linking these requirements to DOE's programs. It also covers independent analysis, developing and maintaining an integrated baseline, hydrogen infrastructure modeling and simulation, configuration control and management, integrating scheduling, budgets, scope of work, and other important areas.

NREL supports the President's Hydrogen Fuel Initiative in many ways, some new and some long-standing. It performs basic research and development in numerous hydrogen areas, verifies the performance of hydrogen technologies in development, validates emerging technologies, and helps establish codes and standards for hydrogen safety.

The Laboratory leads nationwide R&D efforts in:

- production of hydrogen from renewable energy sources;
- delivery and storage of hydrogen in a national infrastructure;
- uses of hydrogen in fuel cells, both in stationary and transportation applications; and
- validation of emerging technologies.

Dale A. Gardner joined NREL on December 1, 2003 to direct the Laboratory's hydrogen systems integration work



**Dale Gardner directs the Laboratory's hydrogen systems integration work for the DOE.**

for the U.S. Department of Energy. The work he leads will directly inform Steve Chalk, manager of DOE's Hydrogen, Fuel Cells and Infrastructure Program.

Gardner came to NREL from Northrop Grumman Mission Systems, where he managed the company's operations in Colorado

Spring, Colorado. He has more than 30 years of experience with industry, NASA, and the military in systems management, design, development, and integration. He began his career with the Navy and the Naval Air Test Center and flew on two space shuttle missions as a mission specialist. Gardner supervised implementation of a worldwide space-sensor network at U.S. Space Command in Colorado Springs before managing engineering support programs for TRW, Inc. and Northrop Grumman Corp.

### **Computational Sciences Center Aids R&D**

Along with theory and experiment, computation is considered an equal and indispensable partner in advancing scientific knowledge and engineering practices. Enormous computational capacity is needed to study the details of complex systems at ever-higher levels of detail and realism.

Recognizing this, NREL has taken several steps toward establishing a first-class computational capability. First came its Computational Sciences Initiative, adopted in 2000. It is a Lab-wide commitment to establish appropriate levels of computing power, data storage, applications software, and skilled support to all centers in the Laboratory. Next was the creation of the Computational Science Center. Situated in Building 16 in Golden, Colorado, the center has five staff members.



**Dr. Steven Hammond directs NREL's Computational Sciences Center.**

Its director is Steve Hammond, who joined NREL in March 2002.

Shortly thereafter came the installation of a supercomputer: a 64 processor IBM SP parallel computer with 64 gigabytes of total memory and a peak speed of 96 billion floating point operations per second (gigaflops). The system is similar in character to machines at Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center.

Equipment such as this is essential to many NREL scientists, says Hammond. "It enables them to study complex systems and natural phenomena in a virtual environment that would otherwise be too expensive or dangerous, or even impossible, to study by direct experimentation." Scientists from NREL's Basic Sciences Center, for example, use the IBM system to simulate and model the electronic structure of materials for PV devices and hydrogen storage.

Hammond came to NREL from the National Center for Atmospheric Research in Boulder, Colorado, where he managed the Computational Sciences Section and led a number of R&D efforts to improve the computational efficiency of climate models. He holds a Ph.D. in Computer Science from Rensselaer Polytechnic Institute in Troy, New York, and master and undergraduate degrees from the University of Rochester.

# Patents

**Method for Improving the Durability of Ion Insertion Materials**, Se-Hee Lee, et al, U.S. Patent 6,420,071, July 16, 2002.

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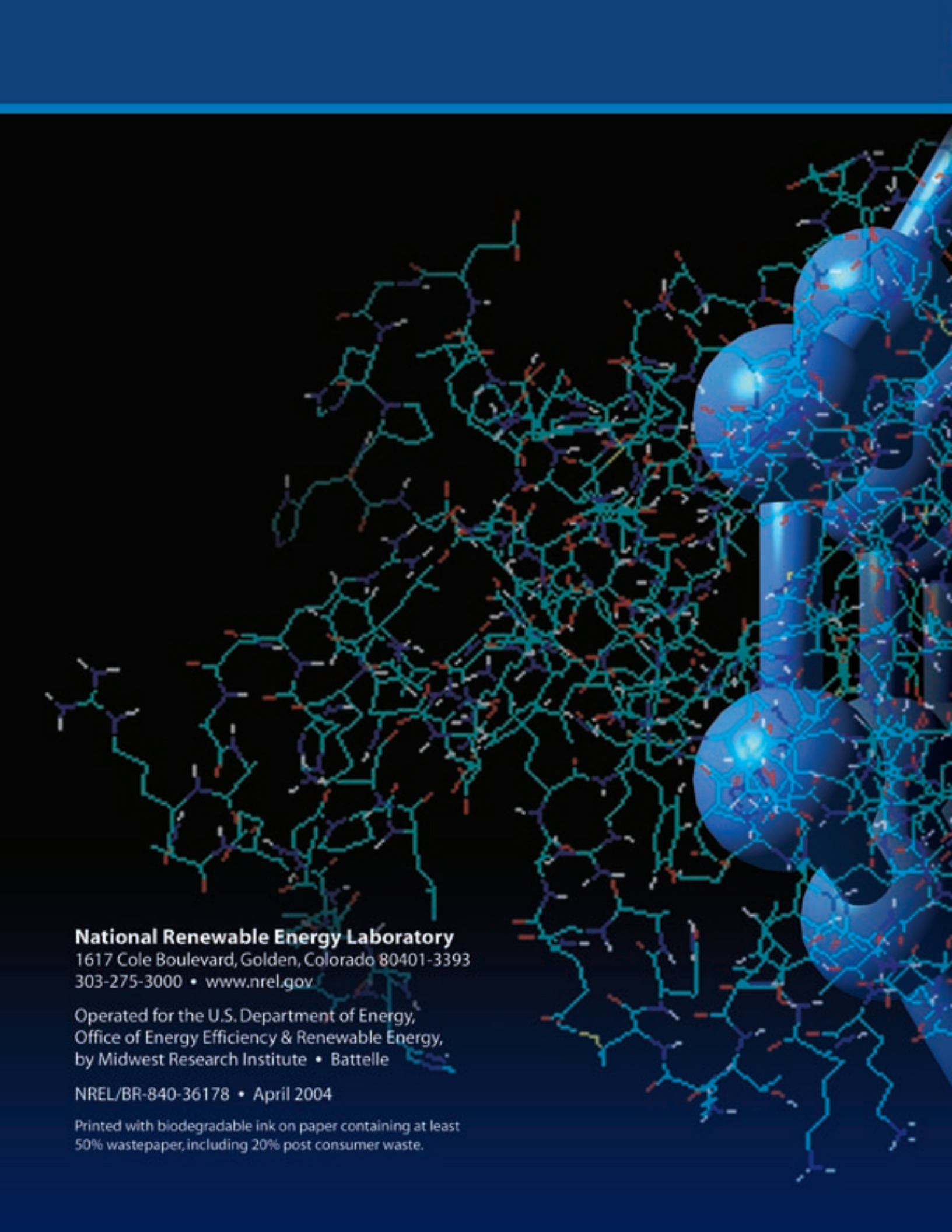
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