ENERGIZING RESEARCH

Are new materials the key to sustainability?

IN THE SEARCH FOR NEW SUSTAINABLE ENERGY TECHNOLOGIES, ANSWERS OFTEN LIE NOT IN DEVICES BUT IN THE MATERIALS THAT MAKE THEM WORK. IN EVERYTHING FROM PHOTOVOLTAIC CELLS TO FUEL CELLS AND ELECTRODES IN BATTERIES, RESEARCHERS ARE LOOKING AT MATERIALS—HOW THEY ACT UNDER DIFFERENT CIRCUMSTANCES, AND HOW THEY CAN BE DESIGNED—TO FIND NEXT-GENERATION SOLUTIONS TO OUR GROWING ENERGY PROBLEMS.
Academia in McCormick’s Department of Materials Science and Engineering have been focusing on the problem of sustainable energy for decades. As funding for energy research increases, McCormick efforts in the area have grown dramatically. Now 49 percent of the department’s research expenditures involve energy research, with projects covering everything from theory to experimentation to characterization. Mark Hersam, Scott Barnett, and Chris Wolverton—all professors of materials science and engineering—are among the many leaders in the search for the materials that will drive new energy technologies.

**Putting Fuel Cells into Reverse**

To create electricity, many power plants take a fossil fuel, burn it to create heat, and use that heat to run an engine that drives a turbine that finally creates electrical energy. It’s a long process that results in an efficiency rate of only about 30 percent.

Scott Barnett, professor of materials science and engineering sees a better way: fuel cells. For 20 years Barnett has researched fuel-cell technology to improve the production of electricity. Fuel cells use an electrochemical reaction to produce electricity directly from the fuel and work by exploiting the reaction between oxygen and hydrogen. By combining hydrogen from a fossil fuel directly with oxygen, it is possible to harness the electricity from the reaction with an efficiency of 40 to 60 percent, nearly twice the efficiency of conventional power plants. Fuel cells also have a much lower rate of carbon dioxide emission.

“The technology has come a long way,” Barnett says. “Fossil fuels like coal are going to be in use for a long time to come, until renewable energy sources take over, and fuel cells provide a means for using them more efficiently and reducing our production of CO₂.”

So why aren’t fuel cells used more often? NASA has used them on its space shuttles, and Google uses fuel cells to power part of its private headquarters. But the cells are still relatively expensive, and most can’t yet be used directly with fossil fuels. Little is known about their durability or lifespan or whether their cost can be reduced enough for broad commercial markets.

Barnett’s work has focused on answering some of those questions by better understanding how a fuel cell works, engineering better materials to improve efficiency, and even using fuel-cell technology for new application, such as energy storage.

Over the last five years Barnett and his research group have been using special microscopy techniques to peer inside fuel cells to see just how they work. Barnett’s team, working with Peter Voorhees, the Frank C. Engelhart Professor of Materials Science and Engineering, spent several years trying to figure out the process for imaging the fuel cells—no one had ever done it before. The process they have settled on works like an MRI: a microscope produces 3-D images that show the inside of a fuel cell, revealing its electrochemical processes.

“Being able to accurately measure these structures is useful in figuring out how they actually work,” Barnett says. “We’re trying to get a handle on how fuel cells degrade over time, and we can do that with this technique. That will allow manufacturers to make better fuel cells in the future.”

More recently, Barnett’s group has explored ways to use fuel cells for energy storage. As people use more and more renewables in the energy grid, one of the big issues is that these sources are intermittent in nature. For instance, solar energy is produced during the day, which doesn’t match consumption patterns. “You have to have some way of storing the electricity,” Barnett says.

In order to use fuel cells for energy storage, Barnett is finding ways to
run them in reverse. The idea is that the fuel cells would take in electricity, along with CO\textsubscript{2} and water, then convert it to methane, which could then be stored with the natural gas supply. Since natural gas is easy to store, it can be accessed when energy is needed. “We’ve done a lot of the background calculations to show that it has the characteristics you need for a good energy-storage system. People worry about cost, availability of materials, efficiency, and long-term durability,” Barnett says. “We have predictions that look good but have to be fleshed out in practice.”

UNDERSTANDING BATTERIES
One of Mark Hersam’s earliest engineering courses as an undergraduate focused on energy. That class sparked a new interest that led him to undergraduate research projects working with a professor whose specialty was nuclear engineering. At the time, however, funding for energy-related projects was hard to find. “It was obvious there wasn’t a lot of funding and that it would be difficult to do work in this area,” says Hersam, professor of materials science and engineering, chemistry, and medicine. “I tabled that idea and began working on electronic materials. But I kept my interest in energy research.”

Now Hersam’s early interests in energy are well suited for a new funding environment. Nearly 40 percent of the current research in his lab is related to energy, up from just 5 percent three years ago. “Energy research has really come onto the scene,” he says.

In 2008 Hersam and his group developed a technique called atomic-force photovoltaic microscopy that measures the electrical current of photovoltaic materials using a tiny conductive tip that is just 10 nanometers in diameter. “Using this technique we can see which parts of the solar cell are running at full capacity,” he says. “We can determine what parts are inefficient, diagnose the sources of the inefficiency, and, from that knowledge, deduce what the problem is and refine the materials for future use.”

Hersam is trying to gain a similar understanding of the material structures and chemical reactions that occur within batteries. In particular, he is focusing on the interface between the electrode and the electrolyte solution inside the battery, known as the solid electrolyte interface, or SEI. “The SEI region is poorly understood but widely believed to be critical to the operation of the battery,” he says.

Understanding the function of the battery has important safety implications: there have been several high-profile incidents of lithium ion batteries catching fire or even exploding. As these types of batteries are used in a wide variety of applications—including powering electric vehicles—it is critical to understand and predict the reactions that take place within the batteries.

Studying the SEI is a challenge. Microscopy techniques are typically conducted in pristine conditions inside ultrahigh-vacuum chambers. To study the battery, however, Hersam and his team must examine the interface while it is submerged in a highly corrosive, flammable electrolyte solution.
Typically we don’t even want air to touch what we’re analyzing, let alone a corrosive material,” he says. “Moving into a complicated, corrosive electrochemical environment isn’t trivial. But it’s an important challenge for microscopy to operate in real environments, especially where energy processes occur.”

Hersam and his team have adapted their equipment to handle the corrosive electrolyte solution. They conduct experiments in a glovebox, allowing atmospheric control of the sample. These techniques allow them to open up the battery and measure the currents at the SEI.

“Within the battery we can see ‘hot spots’ where the chemistry is happening quickly and perhaps uncontrollably,” he says. “We can pinpoint and diagnose failure points. That understanding gives us a fighting chance to engineer a solution to those problems.”

SCREENING MATERIALS FOR SOLAR ENERGY

While many faculty members have added energy-related research to their portfolios as a result of increased research funding, Chris Wolverton has long devoted all of his research to materials with applications in energy—research that is entirely theoretical and computational.

“The kind of calculations we can do are on the atomic scale and based on quantum mechanics,” he says. “They’re interesting because, while we’ve known the equations that govern the motion of electrons and solids for some time, we are now realizing the ability to use them to our advantage.”

Wolverton, a professor of materials science and engineering who joined McCormick four years ago after working for Ford Motor Company, uses a combination of improved algorithms and newly available computational power to develop highly realistic simulations of how different materials behave. Those simulations allow his team to screen hundreds or thousands of materials based on the characteristics required for a particular application and even extend to materials that don’t yet exist. Such capabilities can, in collaboration with experimental efforts, accelerate the development of new energy technologies.

One recent project is in the area of solar energy—with a unique approach. “Most people use solar radiation to produce electricity,” he says. “We’re working with a group from Sandia National Laboratories to use heat from solar energy to drive a reaction that could turn water and carbon dioxide into syngas.”

Syngas is a key ingredient in the industrial production of fuels such as synthetic natural gas, synthetic petroleum, and methanol. Synthetic fuel derived from “recycled” atmospheric carbon dioxide with this solar thermal technology is carbon neutral and therefore does not exacerbate global warming as conventional fossil fuels do.

Colleagues at Sandia have developed a process that works by focusing solar energy to heat a reaction chamber to extremely high temperatures. Within the chamber, a wheel made of a type of metal oxide rotates as it is heated and cooled. While the material is exposed to the heat, it vents oxygen and transforms into a reduced form. Back in a cooler environment, that reduced form of the material wants that lost oxygen back and will split other molecules apart to get it. Exposing it to water results in the creation of hydrogen, and exposing it to carbon dioxide results in carbon monoxide; combined, the system provides the necessary components for syngas.

The project is part of Sandia National Laboratories’ “Sunshine to Petrol” project, which is a major initiative at the lab. Sandia has already demonstrated the feasibility of the technology, but the efficiency is still lower than needed to be commercially viable. Once optimized, such a system could provide an ideal renewable resource to create synthetic fuels, the combustion of which would contribute no new CO₂ to the atmosphere.

Wolverton and his group are working to define the ideal thermodynamic properties needed for this process and are screening a wide variety of materials to attempt to find an optimal material for the process—a situation that’s common to many sustainable technologies. “A lot of energy problems come down to the fact we don’t have the materials we’d like to have,” he says. “That’s not a peripheral problem. That’s a key problem. The worldwide challenge is to find new materials that enable solutions to these problems.”

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