Zeroing in on natural gas storage

There are 13 million vehicles on the road today that run on natural gas—including many buses in the United States. Thanks to recent discoveries of natural gas reserves, this number is expected to increase sharply. Yet storing natural gas remains a challenge. Researchers know that porous crystals called metal-organic frameworks, with their nanoscopic pores and incredibly high surface areas, are excellent materials for natural gas storage. But with millions of different possible structures, how do we know which one is best?

Until recently the process for answering that question meant painstakingly creating and testing each material in a lab. Now, thanks to a new algorithm created in the lab of Randall Q. Snurr, professor of chemical and biological engineering, researchers can generate and test hypothetical metal-organic frameworks (MOFs) to rapidly zero in on the most promising structures. Using a library of 102 chemical building-block components, the researchers generated more than 137,000 hypothetical MOF structures—a number much larger than the total number of MOFs (approximately 10,000) reported to date by all researchers—and tested them computationally for their ability to store natural gas.

“Our team then synthesized one of the most promising materials and found that it beat the US Department of Energy’s natural gas storage target by 10 percent,” Snurr says. “This is proving to be an exceptionally powerful tool.”

In pursuit of a flexible, affordable solar cell

Imagine a solar-powered tent that could be stuffed into a backpack, or a jacket that could power your iPod. Products like these could never be realized with the stiff, bulky solar cells of today. But soon they could be within reach, thanks to a new solar cell material created by Mark C. Hersam (above right), professor of materials science and engineering, chemistry, and medicine, and Tobin J. Marks, the Vladimir N. Ipatieff Professor of Catalytic Chemistry and professor of materials science and engineering.

Solar cells today are reliant on indium tin oxide, one of the few materials that will allow light to pass into the cell and electricity to pass out. But indium tin oxide has drawbacks: it’s brittle, and it’s made from an increasingly rare element, indium. That could be a problem if demand for solar cells grows.

Hersam and Marks are looking to single-walled carbon nanotubes—tiny, hollow cylinders of carbon just one nanometer in diameter—as a solution. Carbon is abundant, inexpensive, and flexible—perfect for on-the-go solar technology. “With this mechanically flexible technology, it’s much easier to imagine integrating solar technology into everyday life, rather than carrying around a large, inflexible solar cell,” Hersam says.
Rethinking rechargeable batteries

Reducing our dependence on oil is one of the major challenges of the 21st century. Electric-powered automobiles could be a large part of the solution, but before we can make the leap to these more sustainable vehicles, we have to address their major shortcoming: rechargeable batteries. Today’s lithium-ion batteries—the type found in cell phones, iPods, and electric cars—hold too little charge and recharge too slowly to make electric cars an attractive option for most Americans.

But that could be changing. Harold H. Kung, professor of chemical and biological engineering, is one of several McCormick researchers at work on an advanced lithium-ion battery that could power the devices of the future. By developing new materials for the electrode—the positive (cathode) and negative (anode) ends of the battery where charging occurs—Kung is obtaining dramatic results.

“We have developed a material that can extend the charge life of the anode of a lithium-ion battery by 10 times when it is new,” Kung says. “Even after 150 charges, which would be one year or more of operation, it is still five times more effective than the one used in lithium-ion batteries on the market today.” In other words, if coupled with a matching positive electrode, Kung’s redesigned battery could charge a cell phone in 15 minutes and keep it charged for more than a week.

Charge capacity and rate can be explained by the movement of lithium ions within the batteries as they travel between the anode and the cathode. As the charge is drawn out of the battery, the lithium ions move from the anode to the cathode through a liquid known as the electrolyte; as the battery is recharged, the ions make the reverse trip.

In current batteries only so many lithium ions can be packed into the anode and cathode. Anodes—the focus of Kung’s research—are made of layer upon layer of carbon-based graphene sheets, which can accommodate only one lithium ion for every six carbon atoms. This limits the battery’s charge capacity and determines how long its charge lasts.

Kung has found a way to fit more lithium ions into the anode. His design utilizes silicon, which can accommodate much more lithium than graphene can—four lithium ions for every silicon atom. There are difficulties with silicon, however: it tends to fracture due to expansion and contraction during charging. To deal with this instability, Kung sandwiches clusters of silicon between the graphene sheets—getting, in his words, “the best of both worlds” by combining the two materials.

Kung’s team also found a way to speed a battery’s charge rate. How quickly a battery can be recharged depends on how quickly the lithium ions travel from the electrolyte into the anode. In current batteries, that process is slow because the graphene sheets, while extremely thin (just one atom thick), are very wide. In the recharging process, lithium ions must travel all the way to the edges of the graphene sheet before coming to rest sandwiched between and in the middle of the sheets. The result is a sort of ionic traffic jam at the edges of the sheets that slows the charging process. Kung’s solution, published last fall in the journal *Advanced Energy Materials*, is to bore minuscule holes in the graphene sheets. The holes—called “in-plane defects”—speed recharging by up to 10 times.

Kung’s team will next work on the cathode of lithium-ion batteries. “The cathode is the next crucial step,” Kung says. “If we can make improvements there that are cost-effective, we are looking at a quantum improvement in battery performance.” If the team is successful, results may be seen in the market within five years, Kung says—first in smaller batteries and eventually in cars.