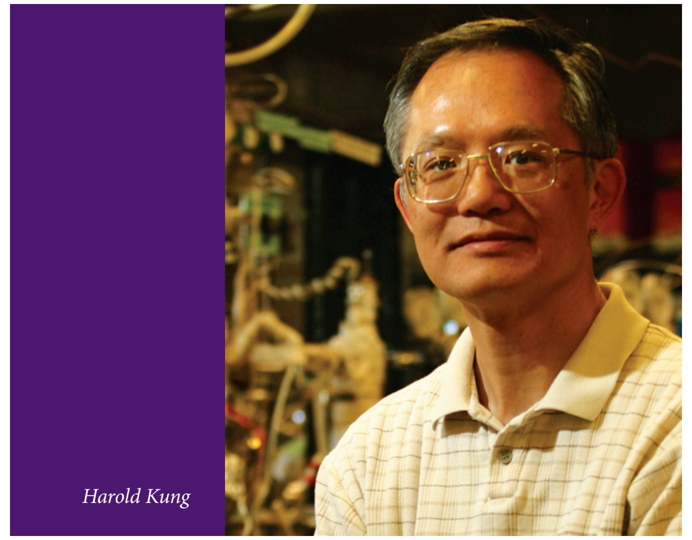
Researchers Design Rechargeable Battery with Improved Charge Capacity, Rate



Harold Kung

Imagine a cellphone battery that stayed charged for more than a week and recharged in just 15 minutes. That dream battery could be closer to reality thanks to McCormick researchers.

A team of engineers has created an electrode for lithium-ion batteries – rechargeable batteries such as those found in cellphones and iPods – that allows the batteries to hold a charge up to 10 times greater and charge 10 times faster than current technology.

The researchers combined two chemical engineering approaches to address two major battery limitations – energy capacity and charge rate – in one fell swoop. In addition to better batteries for cellphones and iPods, the technology could pave the way for more efficient, smaller batteries for electric cars.

> *Imagine a cellphone battery that stayed charged for more than a week and recharged in just 15 minutes.*

A paper describing the research, "In-Plane Vacancy-Enabled High-Power Si-Graphene Composite Electrode for Lithium-Ion Batteries," was published in October by Advanced Energy Materials.

"We have found a way to extend a new lithium-ion battery's charge life by 10 times," said Harold H. Kung, professor of chemical and biological engineering and the paper's lead author. "Even after 150 charges, which would be one year or more of operation, the battery is still five times more effective than lithium-ion batteries on the market today."

Lithium-ion batteries charge through a chemical reaction in which lithium ions are sent between two ends of the battery, the anode and the cathode. As energy in the battery is used, the lithium ions travel from the anode, through the electrolyte, and to the cathode; as the battery is recharged, they travel in the reverse direction.

With current technology, the performance of a lithium-ion battery is limited in two ways. Its energy capacity – how long a battery can maintain its charge – is limited by the charge density, or how many lithium ions can be packed into the anode or cathode. Meanwhile, a battery's charge rate – the speed at which it recharges – is limited by another factor: the speed at which the lithium ions can make their way from the electrolyte into the anode.

In current rechargeable batteries, the anode – made of layers of carbon-based graphene sheets – can only accommodate one lithium atom for every six carbon atoms. To increase energy capacity, scientists have previously experimented with replacing the carbon with silicon, as silicon can accommodate much more lithium: four lithium atoms for every silicon atom. However, silicon expands and contracts dramatically in the charging process, causing fragmentation and losing its charge capacity rapidly.

Currently, the speed of a battery's charge rate is hindered by the shape of the graphene sheets: they are extremely thin — just one carbon atom thick — but by comparison, very long. During the charging process, a lithium ion must travel all the way to the outer edges of the graphene sheet before entering and coming to rest between the sheets. And because it takes so long for lithium to travel to the middle of the graphene sheet, a sort of ionic traffic jam occurs around the edges of the material.

Now, Kung's research team has combined two techniques to combat both these problems. First, to stabilize the silicon in order to maintain maximum charge capacity, they sandwiched clusters of silicon between the graphene sheets. This allowed for a greater number of lithium atoms in the electrode while utilizing the flexibility of graphene sheets to accommodate the volume changes of silicon during use.

"Now we almost have the best of both worlds," Kung said. "We have much higher energy density because of the silicon, and the sandwiching reduces the capacity loss caused by the silicon expanding and contracting. Even if the silicon clusters break up, the silicon won't be lost."

Kung's team also used a chemical oxidation process to create miniscule holes (10 to 20 nanometers) in the graphene sheets so the lithium ions would have a "shortcut" into the anode and be stored there by reaction with silicon. This reduced the time it takes the battery to recharge by up to 10 times.

Other authors of the paper are Xin Zhao, Cary M. Hayner and Mayfair C. Kung, all from Northwestern. The Energy Frontier Research Center program of the U.S. Department of Energy, Basic Energy Sciences, supported the research.

A new, flexible electrode created at McCormick would extend the charge capacity and rate of rechargeable batteries, like those used in cellphones and iPods.

Neda Bagheri Joins ChBE

Neda Bagheri

The Department of Chemical and Biological Engineering welcomes Neda Bagheri, who will join us in February as an assistant professor.

Bagheri completed her studies at the University of California Santa Barbara, receiving her BS in 2002 and her PhD in 2007, both in electrical and computer engineering. Her graduate research, conducted with Professor Francis J. Doyle III, combined control theory with quantitative biological measurements to investigate circadian regulation, structure, and robust phase dynamics. As an undergraduate and graduate student, Bagheri was actively involved with UCSB's Student Entrepreneurial Association and the Center for Entrepreneurship and Engineering Management; she continues to advocate for the translation of engineering research into entrepreneurship, later serving as a consultant for a local start-up company in Cambridge, Mass. Bagheri also had the opportunity to pursue her research abroad, spending much of 2004 as a visiting researcher at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg, Germany.

After completing her PhD, Bagheri conducted postdoctoral research with Professor Douglas A. Lauffenburger at MIT's Department of Biological Engineering, where she integrated experimental and computational studies to investigate cell regulatory dynamics underlying virus-host interaction and immune function. She has published nearly a dozen journal articles and book chapters and has presented at more than 20 conferences and seminars.

Bagheri's career objective is to employ dynamical systems and control theory strategies to address modern challenges in medicine and biology. She is specifically interested in understanding the complex regulatory networks that govern cancer development, immune function, and circadian biology. She looks forward to continuing this research at Northwestern.

Outside the lab, Bagheri enjoys traveling, the arts, and spending time outdoors – especially backpacking, cycling, and rock climbing.

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WINTER 2012

Michael Jewett Receives Prestigious Packard Fellowship

Michael Jewett

Michael C. Jewett, a synthetic biology expert and assistant professor of chemical and biological engineering at McCormick, has been awarded a Packard Fellowship for Science and Engineering by the David and Lucile Packard Foundation.

Jewett is among the 16 promising science and engineering researchers this year nationwide named to receive an unrestricted research grant of $875,000 over five years. These professors are tackling some of the critical scientific questions of our time and promise to have a big impact not just on their fields but also on the students working with them.

With his Packard Foundation funding, Jewett will advance his research on developing cell-free synthetic biology for biomanufacturing new classes of life-saving drugs, sustainable fuels and novel materials from renewable resources, both quickly and on demand.

Jewett was thrilled to receive the Packard Fellowship. "I am honored and excited to be named a Packard Fellow and proud to represent Northwestern and the McCormick School with this achievement," Jewett said. "One of the amazing aspects of this award is the freedom provided by the foundation. My lab has the freedom to explore new directions of research that might be considered too risky by some government funding agencies, especially in today's funding climate."

For decades, scientists have harnessed biology for use as cellular factories to make fuels for cars, antibiotics that fight infections, and targeted therapeutics that attack disease. However, the current approach to engineering cells is often prohibitively costly and remains difficult because of our incomplete knowledge of how life works, Jewett says. And unlike typical engineered systems, cells have their own agenda, such as growth and adaptation.

> *"With the Packard Fellowship, my lab has the freedom to explore new directions of research that might be considered too risky by some government funding agencies." – Assistant Professor Michael Jewett*

Jewett and his team hope to create a new paradigm for engineering biology in the face of these complex challenges. Rather than attempt to balance the tug-of-war between the cell's objectives and the engineer's objectives, they aim to discover efficient new strategies for designing and constructing cell-free systems that transform ensembles of cellular machines such as the enzymes that make protein therapeutics – into systems that can be engineered just as integrated circuits are engineered today.

Linda Broadbelt, chair of the Department of Chemical and Biological Engineering, is enthusiastic about the potential implications of Jewett's research. "The Packard award will enable his research group to lay the intellectual framework for creating a menu of biochemical reactions that can be stitched together in any combination for making new molecules that could touch nearly all aspects of our lives," she said.

Jewett is the first professor in Northwestern's chemical and biological engineering department to earn the fellowship and the second in the McCormick School. The other McCormick recipient is Monica Olvera de la Cruz, the Lawyer Taylor Professor of Materials Science and Engineering.

Other honors received by Jewett this year include the Young Faculty Award from the Defense Advanced Research Projects Agency (DARPA) and the Agilent Early Career Professor Award.

Prior to joining Northwestern in 2009, Jewett made strong contributions to synthetic biology at the Harvard Medical School as a National Institutes of Health Pathway to Independence Award Fellow, to systems biology at the Technical University of Denmark as a National Science Foundation International Postdoctoral Research Fellow, and to cell-free biology during his PhD work at Stanford.

The Packard Foundation invited presidents of 50 U.S. universities to nominate two young professors, each doing innovative research in the natural sciences or engineering. The 16 Packard Fellowship recipients then were chosen from this group.

More Promising Natural Gas Storage?

(From L-R), Graduate student Christopher E. Wilmer and Professor Randall Q. Snurr have developed a computational method that will help scientists zero in on materials that are most efficient for natural gas storage.

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 structures possible, where does one focus?

A McCormick research team has developed a computational method that can save scientists and engineers valuable time in the discovery process. The new algorithm automatically generates and tests hypothetical metal-organic frameworks (MOFs), rapidly zeroing in on the most promising structures. These MOFs then can be synthesized and tested in the lab.

Using their method, the researchers quickly identified more than 300 different MOFs that are predicted to be better than any known material for methane (natural gas) storage. The researchers then synthesized one of the promising materials and found it beat the U.S. Department of Energy (DOE) natural gas storage target by 10 percent.

There already are 13 million vehicles on the road worldwide today that run on natural gas – including many buses in the U.S. – and this number is expected to increase sharply due to recent discoveries of natural gas reserves.

In addition to gas storage and vehicles that burn cleaner fuel, MOFs may lead to better drug-delivery, chemical sensors, carbon capture materials and catalysts. MOF candidates for these applications could be analyzed efficiently using the Northwestern method.

"When our understanding of materials synthesis approaches the point where we are able to make almost any material, the question arises: Which materials should we synthesize?" said Randall Q. Snurr, professor of chemical and biological engineering. Snurr led the research that was published in the journal Nature Chemistry. "This paper presents a powerful method for answering this question for metal-organic frameworks, a new class of highly versatile materials."

Christopher E. Wilmer, a graduate student in Snurr's lab and first author of the paper, developed the new algorithm; Omar K. Farha, research associate professor of chemistry in the Weinberg College of Arts and Sciences, and Joseph T. Hupp, professor of chemistry, led the synthesis efforts.

"Currently, researchers choose to create new materials based on their imagining how the atomic structures might look," Wilmer said. "The algorithm greatly accelerates this process by carrying out such 'thought experiments' on supercomputers."

The researchers were able to determine which of the millions of possible MOFs from a given library of 102 chemical building block components were the most promising candidates for natural-gas storage. In just 72 hours, the researchers generated more than 137,000 hypothetical MOF structures. This number is much larger than the total number of MOFs reported to date by all researchers combined (approximately 10,000 MOFs). The Northwestern team then winnowed that number down to the 300 most promising candidates for high-pressure, room-temperature methane storage.

In synthesizing the natural-gas storage MOF that beat the DOE storage target by 10 percent, the research team showed experimentally that the material's actual performance agreed with the predicted properties.

The new algorithm combines the chemical "intuition" that chemists use to imagine novel MOFs with sophisticated molecular simulations to evaluate MOFs for their efficacy in different applications. The algorithm could help remove the bottleneck in the discovery process, the researchers said.

The Defense Threat Reduction Agency and the U.S. Department of Energy, Office of Science, Basic Energy Sciences, supported the research.

The title of the paper is "Large-Scale Screening of Hypothetical Metal-Organic Frameworks." In addition to Snurr, Hupp, Wilmer and Farha, other authors are Michael Leaf, Chang Yeon Lee and Brad G. Hauser, all from Northwestern.

High-Density Energy Storage Using Self-Assembled Materials: How Does It Work?

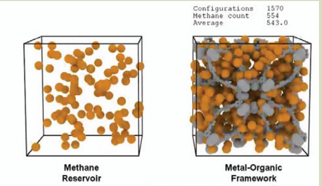
A video by graduate student Christopher E. Wilmer

The problem with fuel tanks today is they can only store liquid fuels, such as gasoline. Gaseous fuels, like methane, are better for the environment — but because gas molecules tend to spread out as far as they can, an ordinary fuel tank would hold very little gaseous fuel. How can we fit more methane inside a tank?

1. Methane molecules, like all gas molecules, are attracted to surfaces, so a tank designed with added surface area would be more effective. For example, a 12-gallon "wall-extension" tank would hold one square meter of methane.

2. But can we do better? A simpler, more effective idea is to fill the tank with sand. Each grain of sand adds a small amount of surface area, but millions of grains of sand fit inside the tank. The result: A sand-filled tank would hold 100 square meters of methane.

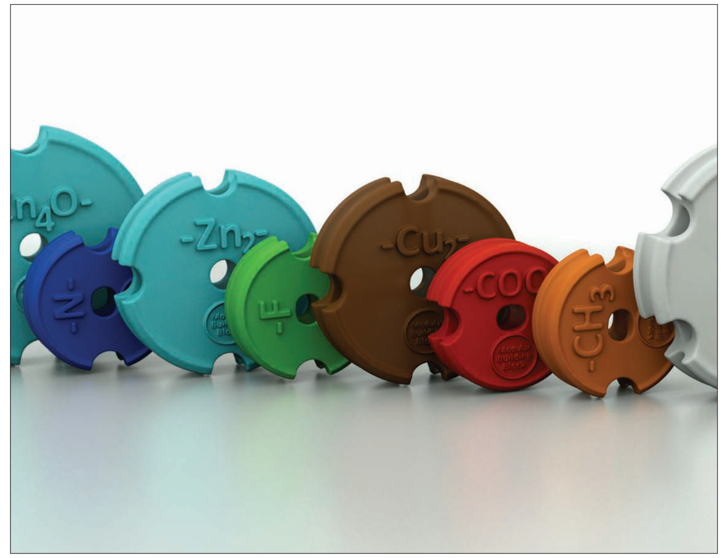
3. Instead of sand, what if we used a material specially designed to accommodate as much methane as possible? Take the self-assembled NU100 crystal, designed at Northwestern University. Each crystal contains trillions of pores, which allows methane to get inside. Filled with these crystals, the same tank would hold 50 million square meters.



4. But do even better materials exist? With thousands of possible combinations, it's difficult to know where to begin — and making each of the materials would take many years. Thankfully, we don't have to make each material; we can now computationally simulate them. We can predict how well a crystal stores methane by connecting it to an imaginary methane reservoir.

To watch the video, visit http://youtube/QaKSekjAnqY

> *"When our understanding of materials synthesis approaches the point where we are able to make almost any material, the question arises: Which materials should we synthesize?" – Professor Randall Q. Snurr*



The algorithm builds MOFs out of molecular pieces by snapping them together as if they were 'Tinkertoys.' These molecular structures can vary significantly in their chemical properties, with each imbuing the assembled MOF with unique capabilities.

Student Successes

Northwestern Team Takes Top Honors at Synthetic Biology Competition

(From left to right): Michael Sherer (biomedical engineering, '13), Valerie Chen (biomedical engineering, '13), Helen Shen (biomedical engineering, '12), Kristin Palarz (biology and integrated sciences, '14), Rafay Faruqi (biomedical engineering, '12), and Nirmit Desai (biological sciences, '13) used E. coli to design a biosensor that can detect the presence of Pseudomonas aeruginosa.

A team of McCormick students took top honors in October at a regional competition for iGEM, an undergraduate synthetic biology competition held at MIT. Their project: an E. coli-based biosensor that could help detect the presence of a harmful bacteria that lurks on hospital faucets and medical equipment.

Participants in iGEM (the International Genetically Engineered Machine competition) are given a kit of biological parts early in the summer from the Registry of Standard Biological Parts, a collection of "mix-and-match" genetic parts.

Students work at their schools over the next several months, using the kits – and new parts they design themselves – to build synthetic biology devices and systems, and operate them in living cells.

"It was very exciting to not only be able to completely design our own project from scratch, but also execute it successfully," said team member Michael Sherer. "It's definitely gotten me interested in continuing research in the future."

Among the team's advisers were chemical and biological engineering professors Michael Jewett, Joshua Leonard, and Keith Tyo.

News & Awards

FACULTY

Luis Amaral joined the editorial board of PLoS ONE and also joined the Faculty of 1000 (F1000), an international faculty of experts who are highly respected in their fields. Members are nominated to the faculty by their F1000 peers.

Linda Broadbelt

Linda Broadbelt is recipient of a 2010/2011 Clarence Ver Steeg Graduate Faculty Award in recognition of her time and effort in support of graduate students.

Wesley Burghardt was selected as a Charles Deering McCormick Professor of Teaching Excellence.

Mike Jewett was awarded the 2011 Agilent Early Career Professor Award and a 2011 DARPA Young Faculty Award.

Chad Mirkin was elected a fellow of the American Academy of Arts and Sciences.

Justin Notestein

Justin Notestein was named a DuPont Young Professor for his work to develop atom-precise materials for heterogeneous catalysis and selective adsorption.

Randy Snurr and **Wes Burghardt** were elected as fellows of the American Association for the Advancement of Science. Professor Snurr was also selected by the American Institute of Chemical Engineers' Board of Directors as recipient of the 2011 Institute Award for Excellence in Industrial Gases Technology.

John Torkelson was selected to the ASG Faculty Honor Roll, which recognizes the 100 best faculty members at Northwestern as voted on by the students.

Fengqi You

Fengqi You was invited to the 9th Annual National Academies Keck Futures Initiative (NAKFI) conference entitled "Ecosystem Services: Charting a Path to Food Security that is a Win-Win for People and the Environment," which was held in November. Professor You was also awarded the 2011 W. David Smith, Jr. Graduate Publication Award given by the Computing and Systems Technology Division of the AIChE for the journal paper: "Design of Responsive Supply Chains under Demand Uncertainty," published in *Computers & Chemical Engineering*.

STUDENTS

Two ChBE students won Undergraduate Research Grants of $3,000 to perform independent research this summer: **Nick Anderson** for his project, "Development of a Primary Mouse Ovarian Follicle in vitro Culture System" (faculty adviser: Lonnie Shea, chemical and biological engineering); and **Charlie Tsai** for his project, "Effect of Crystal Phase Composition and Morphological Properties on the Reductive and Oxidative Abilities of TiO2 Nanotubes under UV and Visible Light" (faculty adviser: Kimberly Gray, Civil and Environmental Engineering and by courtesy, Chemical and Biological Engineering).

Alexander Millard-Swan was awarded first prize in the McCormick Prize competition, recognizing the senior who submits the best insightful, innovative, and/or creative project. His project, "Novel Materials for Sustainability & Energy-Based Applications Enabled by Solid-State Shear Pulverization," was advised by John Torkelson.