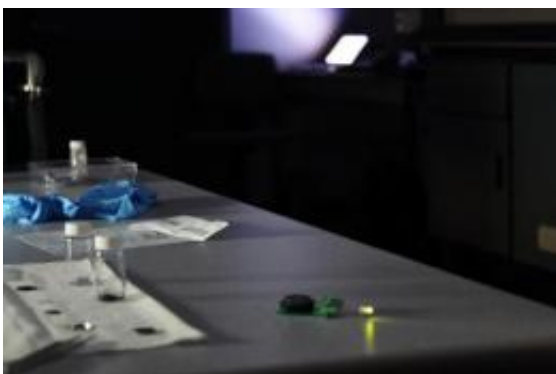


Nanoscale materials for high-energy density lithium-ion batteries

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An experimental battery powers a small yellow light (front, right) in a battery research laboratory run by NanoEngineering professor Shirley Meng at the UC San Diego Jacobs School of Engineering. Photo credit: UC San Diego

(PhysOrg.com) -- NEI Corporation and the University of California, San Diego won a Phase II Small Business Technology Transfer contract from NASA to develop and implement high energy density cathode materials for lithium batteries. These lithium-ion (Li-ion) batteries could be used in a variety of NASA projects - and in a wide range of transportation and consumer applications.

NanoEngineers at the University of California, San Diego are designing new types of lithium-ion (Li-ion) batteries that could be used in a variety of NASA space exploration projects - and in a wide range of transportation and consumer applications. NEI Corporation and UC San

Diego recently won a Phase II Small Business Technology Transfer contract from NASA to develop and implement high energy density cathode materials for lithium batteries.

NEI is the prime contractor on the NASA contract and Shirley Meng, a professor in the Department of NanoEngineering at the UC San Diego Jacobs School of Engineering, is a subcontractor. The nearly \$600,000 program builds upon expertise in the UC San Diego Department of NanoEngineering in modeling new nanocomposite structures for next generation [electrode materials](#), and NEI's capability to reproducibly synthesize electrode materials at the nanoscale.

Battery Applications

Advanced Li-ion battery systems with high energy and power densities - and the ability to operate at low temperatures - are required for NASA's exploration missions. The James Webb Space Telescope (JWST), Mars Atmospheric and Volatile Evolution (MAVEN), deep drilling equipment and Astrobiology Field Laboratory on Mars, International X-ray Observatory (IXO), and extravehicular activities are potential space applications. Advanced lithium-ion battery packs could also be used in hybrid electric vehicles, consumer electronics, medical devices, electric scooters, and a variety of military applications.

Designing Batteries from the Atom Up

The UC San Diego NanoEngineers will help guide development of the new batteries using advanced modeling techniques. "We will give NEI candidate materials that we think will have optimal battery properties, and they will make the materials using their proprietary technology," said professor Shirley Meng, who leads the Laboratory for Energy Storage and Conversion in the Department of NanoEngineering at the

UC San Diego Jacobs School of Engineering.



Batteries on a workbench in the Laboratory for Energy Storage and Conversion run by NanoEngineering professor Shirley Meng at the UC San Diego Jacobs School of Engineering. Photo credit: UC San Diego

The outcome of the program will be a commercially useable cathode material with exceptionally high capacity - more than 250 milliAmp-Hours per gram (250 mAh/g) at about 4V, which translates to an energy density of more than 1000 Watt-hours per kilogram (Wh/kg). This represents a factor of two enhancement in energy density over lithium cobalt oxide, which is the most commonly used cathode material at the present time. NEI expects to have sample cathode materials for testing by interested end-users by the middle of 2011.

The UC San Diego NanoEngineers will design the candidate cathode materials using “first principles calculations” - a quantum-mechanical based calculation method that enables the engineers to predict electrochemical properties of the batteries prior to synthesis.

One aspect of the batteries the engineers will predict is the structural stability of the electrode materials as the lithium concentration fluctuates

during charge and discharge. Enhancing structural stability is critical for extending the life of rechargeable batteries.

“We are pleased to be working closely with Shirley Meng on this exciting materials manufacturing project. The shortest path to developing new materials and implementing them in practical applications is for materials manufacturers to work synergistically with researchers like Prof. Meng, who can create new structures through computation and modeling,” said Dr. Ganesh Skandan, CEO NEI Corporation.

“This work, which could lead to new batteries for space exploration and beyond, is just one example of the high impact research being done in the Department of NanoEngineering,” said Kenneth Vecchio, Professor and Chair of the Department of NanoEngineering at the UC San Diego Jacobs School of Engineering.



The metallic disks are experimental batteries being tested in the Laboratory for Energy Storage and Conversion run by NanoEngineering professor Shirley Meng at the UC San Diego Jacobs School of Engineering. Photo credit: UC San Diego

Batteries for hybrid electric vehicles or full electric cars

Work in the Meng lab on next-generation batteries extends beyond the collaboration with NEI.

“In my group, we are very interested in batteries that will be used in future transportation systems. Lithium batteries for plug-in hybrid electric vehicles or full electric cars have a lot of potential, but we have to work very hard to decrease the dollar per kilowatt hour numbers,” said Meng, whose research group at UC San Diego is funded through grants from the U.S. Department of Energy (DOE) and other government and industry sources.

The new Phase II Small Business Technology Transfer contract follows a similar Phase I contract awarded to the same industry-university team.

“If we are going to use large scale batteries for applications such as electric cars, it is not acceptable to replace batteries every three years. The cycle life of the batteries becomes very important and this is a challenge to address. How do we make batteries last for ten years instead of three years? We have to look for other options for the structure of the battery materials that are more robust,” said Meng.

The Cathode Bottleneck

The positive electrode in lithium-ion batteries - the cathode - is one battery component ripe for additional improvements.

“The cathode is a performance bottleneck for modern lithium batteries that power consumer electronics like PDAs, mp3 players and laptops,” said Meng. “There is plenty of room for improving energy density in lithium batteries by at least another 50 percent. The problem is making these improvements under the constraints of cost. That is the main obstacle. We are looking at dollars per kilowatt hour. We need to make sure the raw materials are low cost, the synthesis process is low cost, and

the packaging of the [battery](#) is low cost,” said Meng.

Moving to Manganese

The lithium ion batteries Meng’s group is working on are primarily manganese based, while most of the [lithium batteries](#) in the marketplace today are cobalt based.

“Manganese is much cheaper than cobalt, and manganese is more abundant,” said Meng. “Also, we are focusing on a different material structure for the batteries, one that is easier to make and could lead to cheaper synthesis.”

The nanoengineers in the Meng lab will be using first principles to model new nanocomposite structures for the generation of [cathode materials](#) with exceptionally high [energy density](#).

“We explore the electrochemical properties of the batteries we design and develop to see if the experimentally measured properties match with our predictions,” said Meng. “We use this feedback mechanism to improve our computational modeling.”

Provided by University of California - San Diego

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