Building a Better Battery

New technologies for sustainable transportation and energy storage

A dead battery isn't only frustrating for mobile phone, tablet and laptop users; energy storage also increasingly impacts transportation. Improved energy storage devices mean increased driving ranges for electric vehicles, which can ultimately reduce carbon dioxide emissions from the transportation sector by lessening its reliance on fossil fuels.

Energy storage for sustainable transportation is top of mind for Assistant Professor **Don Siegel,** who joined the ME faculty in 2009 after working in industry as a researcher at Ford Motor Company. Today, as head of the U-M Energy Storage and Materials Simulation Lab, Siegel is focusing on overcoming the myriad barriers to high-density energy storage using the tools of computational materials science and high-performance computing.

LOOKING TOWARD NEW AND SAFER BATTERY CHEMISTRIES

Through a number of collaborative initiatives, Siegel is looking at both the fundamental science and translational opportunities for new battery technologies. These include his participation in two centers funded by the U.S. Department of Energy: the U.S.-China Clean Energy Research Center-Clean Vehicles Consortium (CERC-CVC) and the Joint Center for Energy Storage Research (JCESR), a public-private energy innovation hub. Both centers are tasked with investigating critical technical questions on the way to developing new energy storage technologies.

The projects in Siegel's lab also are supported by the National Science Foundation—he is a recent CAREER Award winner; see related story on page 11—as well as industry leaders Bosch, Ford and Denso Corporation. "With these research partners, we look at everything from new battery chemistries to improving 'here and now' lithium-ion technologies," he explained.

As an example of the latter approach, Siegel's lab is exploring the chemical reactions underlying safety issues in Li-ion batteries. Specifically, he is investigating electrolyte decomposition at the liquid/solid interfaces between the electrolyte and cathode, a complex interface that has yet to be fully understood (see figure 1). What is known, however, is that electrolyte decomposition at this interface can lead to the accumulation of gases that, when vented to the atmosphere, release highly flammable vapor. Understanding the reaction pathways that precede these safety events will help Siegel and colleagues develop strategies to mitigate them.

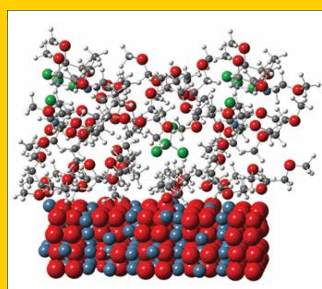

FIGURE 1: Quantum-mechanical simulation of an electrolyte/electrode interface in a Li-air battery.

IDENTIFYING MATERIALS FOR THE STORAGE AND CAPTURE OF GASES

While batteries store energy in the form of electrons, the chemical bonds of molecules also can store energy. In this regard, hydrogen and methane are attracting attention as alternative fuels. Hydrogen is being explored for use in fuel cell vehicles; methane is the primary component of natural gas, which, due to the emergence of hydraulic fracturing, has gained prominence as a low-cost domestic fuel.

However, just as in batteries, achieving high energy densities with either of these fuels is a challenge. Both are gases at standard conditions, and gases typically have very low densities. This results in the same type of "range anxiety" typical for battery electric vehicles.

To address the density problem, hydrogen and natural gas are usually stored on vehicles in compressed or liquefied form, but this approach comes at a cost. "Compression and liquefaction can be expensive and inefficient," explained Siegel, who is looking to develop new materials that could store these gases much more efficiently. "It's a materials discovery challenge to identify new compounds that can store these gases at high densities, and do so at lower pressures and costs."

Siegel's group uses a combination of data mining and high-throughput calculations to identify promising substances from more than half a million candidate compounds stored in the Cambridge Structure Database. By searching this database his team recently identified a handful of porous materials called metal-organic frameworks, or MOFs, that show promise for high-density storage of hydrogen and methane. The findings were published in *Chemistry of Materials* in 2013 (see figure 2).

The search is guided by geometric factors (such as surface area and density), composition and other parameters, but ultimately has to deal with missing or incomplete crystal structures. "Discovering these materials is akin to finding a needle in a haystack—with the important exception that sometimes the needle we find is broken," Siegel said.

While some of the data can be repaired, there remains more to do, both in terms of refining the search and improving the predictions of the amount of hydrogen and methane a given material can store. Nevertheless, the initial successes have attracted attention. "Now some of our experimental colleagues are attempting to synthesize these materials in hopes that they may realize the promise," he said.

CONNECTING RESEARCH TO SOCIETAL IMPACT

Outreach is a large part of Siegel's efforts. To illustrate the linkages between energy policy and the science of energy storage, Siegel developed a series of nine YouTube videos titled "Batteries of the Future." The videos, developed as part of the MconneX program, have been viewed more than 150,000 times and led to several speaking invitations and other connections (see figure 3).

"I believe the videos are helpful because they connect the research students are doing in the lab with their hoped-for consequences. I always encourage students to consider the bigger picture: Why is this work important, and how does one translate from the intended application to the properties that the active material must exhibit?" Siegel said.

For summer 2015, Siegel plans to further extend his outreach activities by developing a weeklong module on energy storage for the U-M Women in Science & Engineering-Girls in Science & Engineering (WISE-GISE) Summer Camp. He's also adding a segment on Battery Safety to a short course he developed for practicing engineers for the College of Engineering's Integrated Systems + Design Certificate in Emerging Automotive Technologies.

A highly sought-after speaker for lay and engineering audiences alike, Siegel was named one of four 2014 National Academy of Engineering Gilbreth Lecturers. He spoke on "Energy Storage for Sustainable Transportation" during the NAE National Meeting in February to an audience comprising both NAE members and high school students.

more on the web

View Siegel's "Batteries of the Future" video series at: **goo.gl/L1VVo**

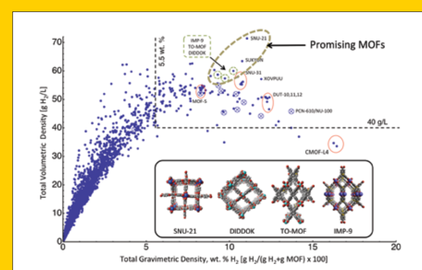

FIGURE 2: High-throughput computational screening of more than 4,000 candidate hydrogen storage materials identifies several "overlooked" MOFs having both high volumetric and gravimetric hydrogen densities. The DOE storage targets are indicated with a dotted line.

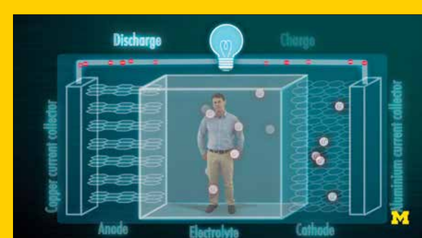

FIGURE 3: Screen-grab from Siegel's YouTube video series, "Batteries of the Future."