SANDIA RESEARCH TO IMPROVE TRANSPORTATION ENERGY STORAGE

Sandia's transportation energy storage research programs apply our scientific understanding of battery degradation mechanisms to develop technologies to improve battery performance, economics, and safety to enable widespread electrification of the nation's transportation fleet.

Automobile and truck transportation accounts for about two thirds of U.S. oil use† and ¼ of our greenhouse gas (GHG) emissions. A national energy goal is to reduce CO2 emissions to 17% of 2005 levels by 2050.‡ Assuming linear growth from today's [population levels and energy-use activities that lead to] emissions, we must achieve over a factor of seven reduction in CO2 emissions. Additionally, the nation would like to reduce petroleum usage for transportation by 17% at the end of this decade.‡

A demonstration Ford Escape PHEV in New York City.

Efficient transportation will be a key element of any path toward reducing oil use and GHGs. Cost-effective emission reductions will be achieved through a combined strategy of improving vehicle engine efficiency, expanding the use of low-net-carbon fuels, and vehicle electrification while enhancing vehicle aerodynamics and reducing vehicle weight. While hybrid and full vehicle electrification improves efficiency, current battery technology imposes range/mobility limitations consumers are reluctant to accept.

Battery safety is a critical factor to battery technology's widespread adoption in the marketplace (via plug-in hybrid electric vehicles [PHEVs] and electric vehicles [EVs]). Any safety issues resulting from poorly designed vehicle batteries could destroy consumer confidence in PHEVs/EVs and set back transportation fleet electrification by years or even decades. Sandia's decades of experience in applied materials R&D and systems and abuse testing assists industry in implementing advanced, science-based safety features that can avoid such incidents.

Sandia researchers are working to create a science-based understanding of electrochemical atomic/molecular processes and connect them with the macroscopic response of packaged batteries to mitigate safety concerns, extend battery lifetimes, and increase battery efficiency through three highly coordinated thrusts:

- large-scale battery testing to measure critical end-of-life mechanisms,
- in situ nano-scale characterization to gain an atomistic understanding of these mechanisms, and
- multi-scale modeling, building predictive models linking atomistic processes with macroscopic responses.

These thrusts, working in conjunction with materials and systems from industry partners, will enable the predictive simulations of battery performance so critically needed to increase battery material capacity, lifetime, and safety.

LARGE-SCALE BATTERY TESTING

Sandia plays a leading role in assuring that lithium-ion batteries are safe and can operate for long periods of time. Sandia obtains batteries/battery materials from research laboratories and battery manufacturers. Sandia researchers study the materials' stability and response to abuse, flame-retardant performance, the high-temperature integrity of separators between the cathode and anode, the mechanisms that initiate internal short circuits and how to mitigate them, and general thermophysical properties.

† U.S. Energy Information Administration, "Annual Energy Review 2009," p. 37
‡ U.S. Department of Energy, "Strategic Plan," May 2011, p. 9–10.

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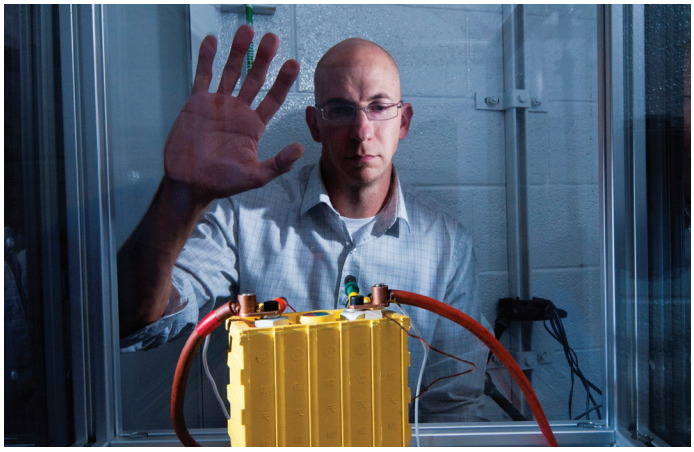


A Sandia researcher prepares to test a battery to determine its response under abuse conditions.

Sandia is the independent abuse testing laboratory for the DOE and the U.S. Advanced Battery Consortium. Its work is helping to develop batteries that have a graceful failure—meaning that if a battery is damaged, it's failure won't cause other problems. To achieve this goal, Sandia has been able to understand and quantify mechanisms that lead to poor abuse tolerance, including heat- and gas-generating reactions. Understanding the chemical response to abuse points the way to improved ~~battery materials~~.

Our Battery Abuse Testing Laboratory, has the capabilities for fundamental characterization of reaction mechanics that lead to safety issues, calorimetry tools to quantify heat generation in batteries, and facilities to accommodate testing larger PHEV and EV battery packs.

CHARACTERIZING CHEMISTRY AND MATERIALS RESPONSE AT THE ATOMIC SCALE

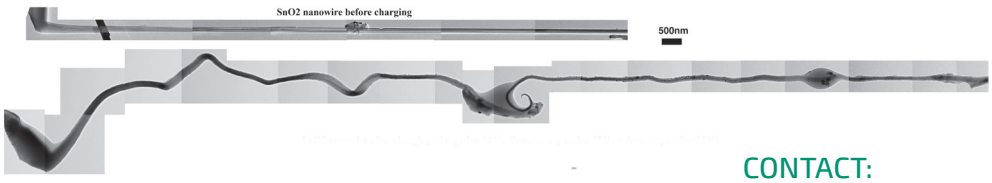
In recent years, the industry/research community has achieved significant improvement in anode/cathode behavior and energy density (particularly on the cathode side). To complement these electrode advances, Sandia is working on several electrolyte development programs with the overall goal of improving electrolyte safety. Increasing the energetic content of a battery increases the focus on safe and reliable performance. We are applying Sandia's science and technology capabilities to address mechanisms associated with battery failure.

The Center for Integrated Nanotechnologies capabilities take this characterization effort to the nano scale. Recently, researchers formed a lithium-ion nanowire inside a transmission electron microscope—giving them the ability to directly observe changes in atomic structure during charging/discharging. What they found—that the wire increased in length much more than it increased in diameter—directly contradicted the prevailing belief. This result has significant implications for the stress a battery experiences—and how many charge/discharge cycles it can endure. Developing an understanding of materials' physical changes during charge/discharge can lead to improved electrode architecture, enabling improvements in efficiency, energy density, reliability, safety, and lifetime.

PREDICTIVE MODELS LINKING ATOMISTIC PROCESSES WITH MACROSCOPIC RESPONSES

Understanding the complex mechanisms that lead to battery failure are important to improving safety and reliability. We are developing a physics-based numerical simulation capability rooted in a first-principles description of the governing atomistic processes. The atomistic chemical information will be propagated through multiple length scales to a continuum-scale description of the battery's electrochemical dynamics.

This simulation capability will enable Sandia to explore and characterize a variety of operational conditions to identify potential safety and stability issues of new battery designs and mitigate them before a battery is designed. This will constitute a unique capability with far reaching value for Sandia's work in battery technology and energy systems for government sponsors and commercial partners.



SnO2 nanowire after charging, elongation 90%. diameter expansion 35%, volume expansion 250%

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