To enhance the nation’s security and prosperity through sustainable, transformative approaches to our most challenging energy, climate, and infrastructure problems.

Automobile and truck transportation accounts for 71% of U.S. oil use and 33.5% of 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, 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.

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 electric vehicle marketplace. Any safety issues resulting from poorly designed vehicle batteries could destroy consumer confidence in plug-in hybrid electric vehicles (PHEVs) and electric vehicles (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’s goal is a science-based understanding of electrochemical atomic/molecular processes that is connected with the macroscopic response of packaged batteries to mitigate safety concerns, extend battery lifetimes, and increase battery efficiency through three highly coordinated thrusts:

1. **large-scale battery testing** to measure critical thermochemical and thermophysical response phenomena that can provide detectable signatures of end-of-life degradation mechanisms,
2. **in situ nano-scale characterization** to gain an atomistic understanding of these mechanisms, and

These thrusts, using commercial 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 and battery materials from research laboratories and battery manufacturers. Sandia researchers study the materials’ stability and response to abuse, flame-retardant performance, the high—

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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.

Sandia has capabilities that take this characterization effort to the nano scale. For example, researchers at Sandia's Center for Integrated Nanotechnologies have 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 understanding the stresses a battery experiences and how many charge/discharge cycles it can endure. Developing an understanding of physical changes during charge and discharge can lead to improved electrode architectures, enabling improvements in cost 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.

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SnO₂ nanowire before charging

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