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Batteries of the Future: Modeling Lithium-ion Battery Behavior

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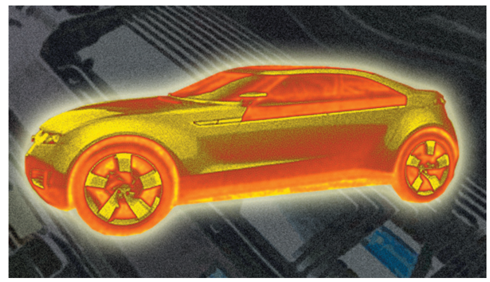
The BATT Program (Batteries for Advanced Transportation Technologies) is a $6 million Department of Energy program that aims to develop next-generation batteries for use in electric, hybrid-electric (HEV), and plug-in hybrid-electric vehicles. Berkeley Lab's Environmental Energy Technologies Division (EETD) assists DOE in managing research conducted under this program, which takes place at Berkeley Lab, other national labs, universities, and private companies.



The future success of electric vehicles like the Chevy Volt pictured here will depend upon greatly improved battery power and energy.

The next generation of batteries in your car is coming from laboratories—and from computer models too. Advanced battery development is no longer just a question of trial and error engineering; scientists increasingly use computer models to design the best possible battery.

Experts consider batteries based on lithium the most promising, in part because of their high voltage—as much as 3.7 volts, as compared to 2.0 volts for a lead-acid battery or 1.2 volts for a nickel metal hydride cell. This high voltage translates directly into higher energy, which has been key to commercializing lithium ion (Li-ion) batteries for cellphone and laptop applications.

Lithium batteries "allow for significant improvements in presently available HEVs," says Venkat Srinivasan, a staff scientist in EETD. "In addition, it is hoped that lithium batteries will pave the way for the development of plug-in HEVs and the electric vehicles of the future."

For lithium batteries to become widespread in vehicles, however, their performance and life need to improve, their safety must be enhanced, and their costs need to decline. "Pure electric vehicles will be a major challenge," Srinivasan says; even fuel-cell vehicles will need high-performance batteries for acceleration.

"The choice of materials for the anode, cathode, and electrolyte has a major impact on the various problems facing lithium batteries today," Srinivasan explains. "Even after a decade of research, no magic combination of material has been found that has all the good attributes."

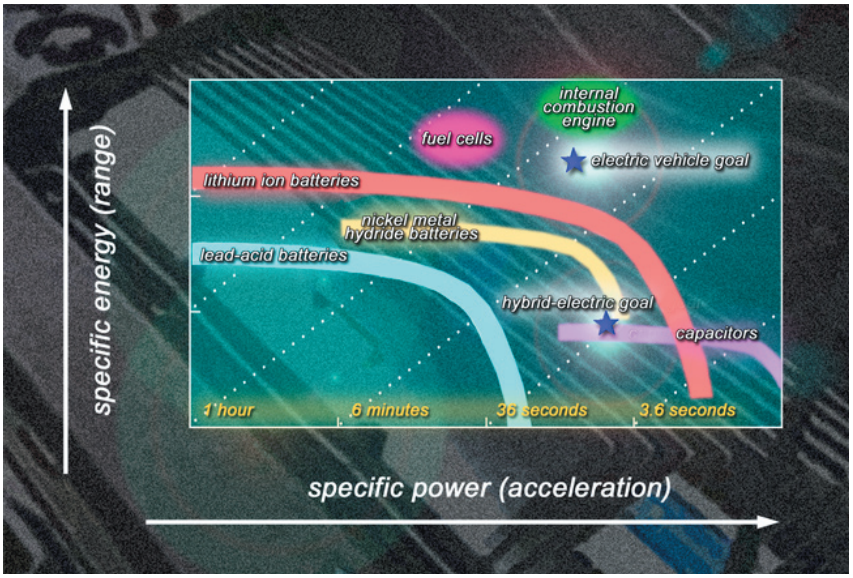
EETD researchers study batteries in many different ways, including synthesizing new anodes, cathodes, and electrolytes; fabricating test batteries with advanced materials and measuring their performance in the lab; understanding their behavior using advanced diagnostics, including microprobe techniques; and creating computer models of battery behavior.

This last is the approach taken by Srinivasan, who works in EETD's Electrochemical Technologies Group. He uses mathematical models of battery chemistry to evaluate the performance limitations of particular Li-ion chemistries. He simulates the performance of a particular chemistry and compares it to experiments performed in the lab to see how well his model results hold up. From the results he extracts information about what factors in a particular material are limiting the performance of the battery. Material developers and battery engineers can use the information to design a better battery that comes closer to meeting the needs of real applications.

"If the model shows that the material looks promising for, say, a plug-in HEV," Srinivasan says, "then we can spend the time and effort to make large amounts of this material, make prototype batteries with it, and see how they will perform in the real world." What particularly interests Srinivasan about the work "is that I can connect the materials-development scientists with those who are optimizing the batteries, and I can make this connection quickly."

Acceleration and range

Srinivasan charts the current performance of batteries and other technologies—and where they have to go to be useful for electric vehicles—in map form. The horizontal axis, power, represents acceleration; for acceleration comparable to internal combustion engines, electric cars need to be able to ramp up power quickly. The map's vertical axis is the amount of energy a battery can store. It's a measure of range—the more energy the battery stores, the farther the car can travel.



A map developed by Venkat Srinivasan from product fact sheets compares the specific energy (in watt-hours per kilogram) of vehicle power sources, an indicator of their range, with their specific power (in watts per kilogram), an indicator of acceleration. Dotted lines show acceleration and cruise times, while blue stars show DOE's energy and power goals for electric vehicles and hybrids. Internal combustion engines still out-perform all other power sources, but battery researchers are confident they can improve the profile of lithium-ion batteries.

Different types of batteries are represented on the map by curved lines showing the decrease in stored energy as power increases. All batteries show a big decline in energy—that is, range—as they achieve more power, or acceleration.

A star on the lower right of the map represents DOE's goal for hybrid electric vehicles. Some lithium-ion batteries on the market today already meet the goal, but while they provide sufficient acceleration, their range is limited. Nickel metal hydride batteries fall short, and lead acid batteries, the oldest of all technologies, trail the pack.

The upper star on the map represents DOE's range and acceleration goal for future electric vehicles. No batteries currently match the performance of internal combustion engines, although lithium-ion batteries come closest. Fuel cells could theoretically approach the range and acceleration needs of electric vehicles, but this technology is unproven.

From real batteries to models and back again

Srinivasan models lithium-ion materials sent to Berkeley Lab from groups throughout the world. He and other Berkeley Lab researchers perform tests to compare similar battery chemistries from different sources. Particularly promising are compounds of lithium iron phosphate with graphite, an electrically conductive form of carbon.

Srinivasan's model can tell whether differences in performance are caused by a battery's design or by something intrinsic to the material itself. "This is what I love about batteries," he says. "Each one has its own idiosyncrasies; there's something a little different about each battery chemistry. To get the right physics, you have to keep adding more details."

Says Srinivasan, "My hope is that five years from now, we will have a plug-and-play model for these battery materials. We are not at that stage right now," but he notes that computer models have gotten better over the years. Interest in batteries has led to increased funding and more people studying the problems. "You need a critical mass of researchers thinking about batteries every day to make progress."

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