Designing better batteries for electric vehicles

August 17 2021, by Nancy W. Stauffer

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The urgent need to cut carbon emissions is prompting a rapid move toward electrified mobility and expanded deployment of solar and wind on the electric grid. If those trends escalate as expected, the need for better methods of storing electrical energy will intensify.

"We need all the strategies we can get to address the threat of climate change," says Elsa Olivetti Ph.D. '07, the Esther and Harold E. Edgerton Associate Professor in Materials Science and Engineering. "Obviously, developing technologies for grid-based storage at a large scale is critical. But for mobile applications—in particular, transportation—much research is focusing on adapting today's lithium-ion battery to make versions that are safer, smaller, and can store more energy for their size and weight."

Traditional lithium-ion batteries continue to improve, but they have limitations that persist, in part because of their structure. A lithium-ion battery consists of two electrodes—one positive and one negative—sandwiched around an organic (carbon-containing) liquid. As the battery is charged and discharged, electrically charged particles (or ions) of lithium pass from one electrode to the other through the liquid electrolyte.

One problem with that design is that at certain voltages and temperatures, the liquid electrolyte can become volatile and catch fire. "Batteries are generally safe under normal usage, but the risk is still there," says Kevin Huang Ph.D. '15, a research scientist in Olivetti's group.

Another problem is that lithium-ion batteries are not well-suited for use in vehicles. Large, heavy battery packs take up space and increase a vehicle's overall weight, reducing fuel efficiency. But it's proving difficult to make today's lithium-ion batteries smaller and lighter while maintaining their energy density—that is, the amount of energy they store per gram of weight.

To solve those problems, researchers are changing key features of the lithium-ion battery to make an all-solid, or "solid-state," version. They replace the liquid electrolyte in the middle with a thin, solid electrolyte that's stable at a wide range of voltages and temperatures. With that solid electrolyte, they use a high-capacity positive electrode and a high-capacity, lithium metal negative electrode that's far thinner than the usual layer of porous carbon. Those changes make it possible to shrink the overall battery considerably while maintaining its energy-storage capacity, thereby achieving a higher energy density.

"Those features—enhanced safety and greater energy density—are probably the two most-often-touted advantages of a potential solid-state battery," says Huang. He then quickly clarifies that "all of these things are prospective, hoped-for, and not necessarily realized." Nevertheless, the possibility has many researchers scrambling to find materials and designs that can deliver on that promise.

Thinking beyond the lab

Researchers have come up with many intriguing options that look promising—in the lab. But Olivetti and Huang believe that additional practical considerations may be important, given the urgency of the climate change challenge. "There are always metrics that we researchers use in the lab to evaluate possible materials and processes," says Olivetti. Examples might include energy-storage capacity and charge/discharge rate. When performing basic research—which she deems both necessary and important—those metrics are appropriate. "But if the aim is implementation, we suggest adding a few metrics that specifically address the potential for rapid scaling," she says.

Based on industry's experience with current lithium-ion batteries, the MIT researchers and their colleague Gerbrand Ceder, the Daniel M. Tellep Distinguished Professor of Engineering at the University of California at Berkeley, suggest three broad questions that can help identify potential constraints on future scale-up as a result of materials selection. First, with this battery design, could materials availability, supply chains, or price volatility become a problem as production scales up? (Note that the environmental and other concerns raised by expanded mining are outside the scope of this study.) Second, will fabricating batteries from these materials involve difficult manufacturing steps during which parts are likely to fail? And third, do manufacturing measures needed to ensure a high-performance product based on these materials ultimately lower or raise the cost of the batteries produced?

To demonstrate their approach, Olivetti, Ceder, and Huang examined some of the electrolyte chemistries and battery structures now being investigated by researchers. To select their examples, they turned to previous work in which they and their collaborators used text- and data-mining techniques to gather information on materials and processing details reported in the literature. From that database, they selected a few frequently reported options that represent a range of possibilities.

Materials and availability

In the world of solid inorganic electrolytes, there are two main classes of materials—the oxides, which contain oxygen, and the sulfides, which contain sulfur. Olivetti, Ceder, and Huang focused on one promising electrolyte option in each class and examined key elements of concern for each of them.

The sulfide they considered was LGPS, which combines lithium, germanium, phosphorus, and sulfur. Based on availability considerations, they focused on the germanium, an element that raises concerns in part because it's not generally mined on its own. Instead, it's a byproduct produced during the mining of coal and zinc.

To investigate its availability, the researchers looked at how much germanium was produced annually in the past six decades during coal and zinc mining and then at how much could have been produced. The outcome suggested that 100 times more germanium could have been produced, even in recent years. Given that supply potential, the availability of germanium is not likely to constrain the scale-up of a solid-state battery based on an LGPS electrolyte.

The situation looked less promising with the researchers' selected oxide, LLZO, which consists of lithium, lanthanum, zirconium, and oxygen. Extraction and processing of lanthanum are largely concentrated in China, and there's limited data available, so the researchers didn't try to analyze its availability. The other three elements are abundantly available. However, in practice, a small quantity of another element—called a dopant—must be added to make LLZO easy to process. So the team focused on tantalum, the most frequently used dopant, as the main element of concern for LLZO.

Tantalum is produced as a byproduct of tin and niobium mining. Historical data show that the amount of tantalum produced during tin and niobium mining was much closer to the potential maximum than was the case with germanium. So the availability of tantalum is more of a concern for the possible scale-up of an LLZO-based battery.

But knowing the availability of an element in the ground doesn't address the steps required to get it to a manufacturer. So the researchers investigated a follow-on question concerning the supply chains for critical elements—mining, processing, refining, shipping, and so on. Assuming that abundant supplies are available, can the supply chains that deliver those materials expand quickly enough to meet the growing demand for batteries?

In sample analyses, they looked at how much supply chains for germanium and tantalum would need to grow year to year to provide batteries for a projected fleet of electric vehicles in 2030. As an example, an electric vehicle fleet often cited as a goal for 2030 would require production of enough batteries to deliver a total of 100 gigawatt hours of energy. To meet that goal using just LGPS batteries, the supply chain for germanium would need to grow by 50 percent from year to year—a stretch, since the maximum growth rate in the past has been about 7 percent. Using just LLZO batteries, the supply chain for tantalum would need to grow by about 30 percent—a growth rate well above the historical high of about 10 percent.

Those examples demonstrate the importance of considering both materials availability and supply chains when evaluating different solid electrolytes for their scale-up potential. "Even when the quantity of a material available isn't a concern, as is the case with germanium, scaling all the steps in the supply chain to match the future production of electric vehicles may require a growth rate that's literally unprecedented," says Huang.

Materials and processing

In assessing the potential for scale-up of a battery design, another factor to consider is the difficulty of the manufacturing process and how it may impact cost. Fabricating a solid-state battery inevitably involves many steps, and a failure at any step raises the cost of each battery successfully produced. As Huang explains, "You're not shipping those failed batteries; you're throwing them away. But you've still spent money on the materials and time and processing."

As a proxy for manufacturing difficulty, Olivetti, Ceder, and Huang explored the impact of failure rate on overall cost for selected solid-state battery designs in their database. In one example, they focused on the oxide LLZO. LLZO is extremely brittle, and at the high temperatures involved in manufacturing, a large sheet that's thin enough to use in a high-performance solid-state battery is likely to crack or warp.

To determine the impact of such failures on cost, they modeled four key processing steps in assembling LLZO-based batteries. At each step, they calculated cost based on an assumed yield—that is, the fraction of total units that were successfully processed without failing. With the LLZO, the yield was far lower than with the other designs they examined; and, as the yield went down, the cost of each kilowatt-hour (kWh) of battery energy went up significantly. For example, when 5 percent more units failed during the final cathode heating step, cost increased by about $30/kWh—a nontrivial change considering that a commonly accepted target cost for such batteries is $100/kWh. Clearly, manufacturing difficulties can have a profound impact on the viability of a design for large-scale adoption.

Materials and performance

One of the main challenges in designing an all-solid battery comes from "interfaces"—that is, where one component meets another. During manufacturing or operation, materials at those interfaces can become unstable. "Atoms start going places that they shouldn't, and battery performance declines," says Huang.

As a result, much research is devoted to coming up with methods of stabilizing interfaces in different battery designs. Many of the methods proposed do increase performance; and as a result, the cost of the battery in dollars per kWh goes down. But implementing such solutions generally involves added materials and time, increasing the cost per kWh during large-scale manufacturing.

To illustrate that trade-off, the researchers first examined their oxide, LLZO. Here, the goal is to stabilize the interface between the LLZO electrolyte and the negative electrode by inserting a thin layer of tin between the two. They analyzed the impacts—both positive and negative—on cost of implementing that solution. They found that adding the tin separator increases energy-storage capacity and improves performance, which reduces the unit cost in dollars/kWh. But the cost of including the tin layer exceeds the savings so that the final cost is higher than the original cost.

In another analysis, they looked at a sulfide electrolyte called LPSCl, which consists of lithium, phosphorus, and sulfur with a bit of added chlorine. In this case, the positive electrode incorporates particles of the electrolyte material—a method of ensuring that the lithium ions can find a pathway through the electrolyte to the other electrode. However, the added electrolyte particles are not compatible with other particles in the positive electrode—another interface problem. In this case, a standard solution is to add a "binder," another material that makes the particles stick together.

Their analysis confirmed that without the binder, performance is poor, and the cost of the LPSCl-based battery is more than $500/kWh. Adding the binder improves performance significantly, and the cost drops by almost $300/kWh. In this case, the cost of adding the binder during manufacturing is so low that essentially all the of the cost decrease from adding the binder is realized. Here, the method implemented to solve the interface problem pays off in lower costs.

The researchers performed similar studies of other promising solid-state batteries reported in the literature, and their results were consistent: The choice of battery materials and processes can affect not only near-term outcomes in the lab but also the feasibility and cost of manufacturing the proposed solid-state battery at the scale needed to meet future demand. The results also showed that considering all three factors together—availability, processing needs, and battery performance—is important because there may be collective effects and trade-offs involved.

Olivetti is proud of the range of concerns the team's approach can probe. But she stresses that it's not meant to replace traditional metrics used to guide materials and processing choices in the lab. "Instead, it's meant to complement those metrics by also looking broadly at the sorts of things that could get in the way of scaling"—an important consideration given what Huang calls "the urgent ticking clock" of clean energy and climate change.

More information: Rubayyat Mahbub et al, Text mining for processing conditions of solid-state battery electrolytes, *Electrochemistry Communications* (2020). DOI: 10.1016/j.elecom.2020.106860

Kevin J. Huang et al, Manufacturing scalability implications of materials choice in inorganic solid-state batteries, *Joule* (2021). DOI: 10.1016/j.joule.2020.12.001

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