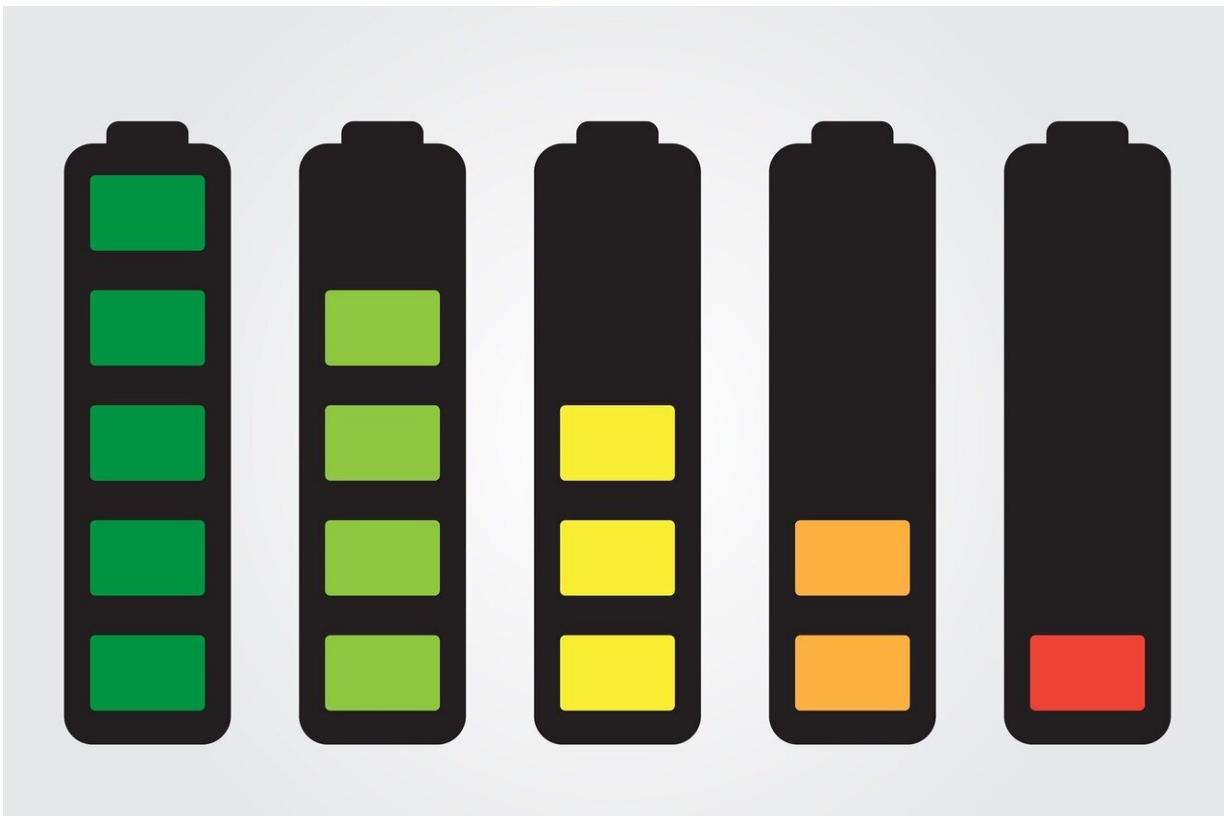


New mathematical model offers potential solutions for next-generation battery challenges

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A new study by Stanford University researchers lights a path forward for building better, safer lithium-metal batteries.

Close cousins of the rechargeable lithium-ion cells widely used in portable electronics and [electric cars](#), lithium-metal batteries hold tremendous promise as next-generation energy storage devices. Compared to lithium-ion devices, lithium-metal batteries hold more energy, charge up faster, and weigh considerably less.

To date, though, the commercial use of rechargeable lithium-metal batteries has been limited. A chief reason is the formation of "dendrites"—thin, metallic, tree-like structures that grow as lithium metal accumulates on electrodes inside the battery. These dendrites degrade battery performance and ultimately lead to failure which, in some instances, can even dangerously ignite fires.

The new study approached this dendrite problem from a theoretical perspective. As described in the paper, published in the *Journal of The Electrochemical Society*, Stanford researchers developed a [mathematical model](#) that brings together the physics and chemistry involved in dendrite formation.

This model offered the insight that swapping in new electrolytes—the medium through which lithium ions travel between the two electrodes inside a battery—with certain properties could slow or even outright stop dendrite growth.

"Our study's aim is to help guide the design of lithium-metal batteries with longer life span," said the study lead author Weiyu Li, a Ph.D. student in energy resources engineering co-advised by Professors Daniel Tartakovsky and Hamdi Tchelepi. "Our [mathematical framework](#) accounts for the key chemical and [physical processes](#) in lithium-metal batteries at the appropriate scale."

"This study provides some of the specific details about the conditions under which dendrites can form, as well as possible pathways for

suppressing their growth," said study co-author Tchelepi, a professor of energy resources engineering at Stanford's School of Earth, Energy & Environmental Sciences (Stanford Earth).

A direction for design

Experimentalists have long strived to understand the factors leading to dendrite formation, but the laboratory work is labor intensive, and results have proven difficult to interpret. Recognizing this challenge, the researchers developed a mathematical representation of the batteries' internal electric fields and transport of lithium ions through the electrolyte material, alongside other relevant mechanisms.

With the results of the study in hand, experimentalists can focus on physically plausible material and architecture combinations. "Our hope is that other researchers can use this guidance from our study to design devices that have the right properties and reduce the range of trial-and-error, experimental variations they have to do in the lab," Tchelepi said.

Specifically, the new strategies for electrolyte design called for by the study include pursuing materials that are anisotropic, meaning they exhibit different properties in different directions. A classic example of an anisotropic material is wood, which is stronger in the direction of the grain, visible as lines in the wood, versus against the grain. In the case of anisotropic electrolytes, these materials could finetune the complex interplay between ion transport and interfacial chemistry, thwarting buildup that proceeds dendrite formation. Some liquid crystals and gels display these desired characteristics, the researchers suggest.

Another approach identified by the study centers on battery separators—membranes that prevent electrodes at opposite ends of the battery from touching and short-circuiting. New kinds of separators could be designed that feature pores which cause lithium ions to pass

back and forth through the electrolyte in an anisotropic manner.

Building and testing

The team looks forward to seeing other scientific investigators follow up on the "leads" identified in their study. Those next steps will involve manufacturing real devices that rely on experimental new electrolyte formulations and battery architectures, then testing out which might prove effective, scalable, and economical.

"An enormous amount of research goes into materials design and experimental verification of complex battery systems, and in general, mathematical frameworks like that spearheaded by Weiyu have been largely missing in this effort," said co-author Tartakovsky, a professor of [energy resources](#) engineering at Stanford.

Following through on these latest results, Tartakovsky and colleagues are working on constructing a fully-fledged virtual representation—known as a "digital avatar"—of lithium-metal battery systems, or DABS.

"This study is a key building block of DABS, a comprehensive 'digital avatar' or replica of lithium-metal batteries that is being developed in our lab," said Tartakovsky. "With DABS, we will continue to advance the state of the art for these promising energy storage devices."

More information: Weiyu Li et al, Stability-Guided Strategies to Mitigate Dendritic Growth in Lithium-Metal Batteries, *Journal of The Electrochemical Society* (2022). [DOI: 10.1149/1945-7111/ac7978](https://doi.org/10.1149/1945-7111/ac7978)

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