# Using magnetic resonance spectroscopy to design safer, higher-performance lithium batteries

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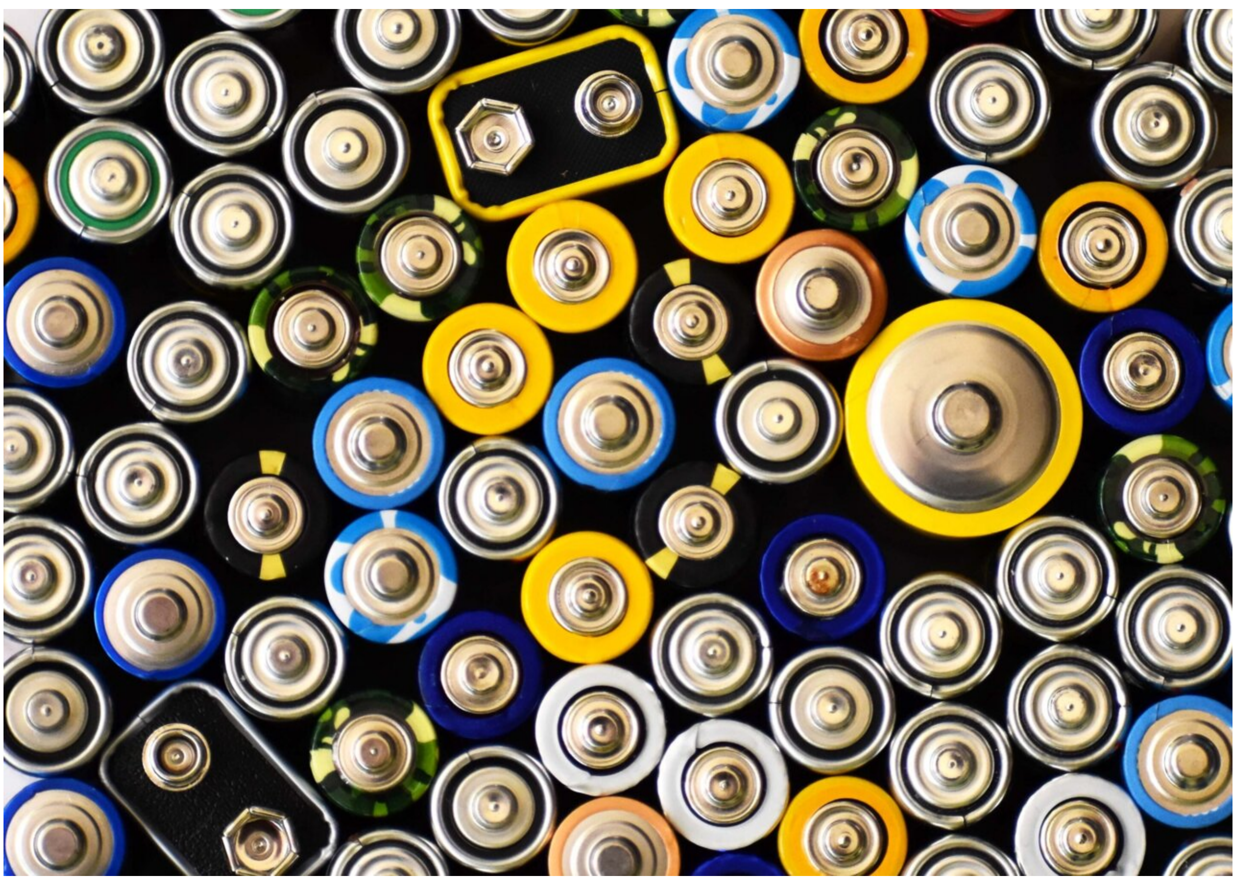

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A Columbia Engineering team has published a paper in the journal *Joule* that details how nuclear magnetic resonance spectroscopy techniques can be leveraged to design the anode surface in lithium metal batteries. The researchers also present new data and interpretations for how this method can be used to gain unique insight into the structure of these surfaces to share with the field.

"We believe that, armed with all the data we've pulled together, we can help accelerate the design of lithium metal batteries and help make them safe for consumers, which folks have been trying to do for more than four decades," said the team's leader Lauren Marbella, associate professor of chemical engineering.

Batteries that use a lithium metal anode instead of a graphite anode, like the ones used in our cell phones and electric vehicles, will enable more affordable and versatile electrified modes of transportation, including semi-trucks and small aircraft. For example, the price of electric vehicle batteries would decrease while simultaneously offering a longer range (from 400 km to >600 km).

## Why they're hard to commercialize

But commercializing lithium metal batteries is still far off in the future. Lithium metal is one of the most reactive elements on the periodic table and readily develops a passivation layer that impacts the structure of the anode itself during normal battery use. This passivation layer is like the layer that develops when silverware or jewelry begins to tarnish, but because lithium is so reactive, the lithium metal anode in a battery will begin to "tarnish" as soon as it touches the electrolyte.

The chemistry of the passivation layer impacts how lithium ions move during battery charging/discharging, ultimately impacting whether or not metal filaments that lead to poor battery performance grow inside of the system.

Up to now, measuring the chemical composition of the passivation layer, known by the battery community as the solid electrolyte interphase (SEI), while simultaneously capturing information on how lithium ions located in that layer are moving around has been next to impossible.

Marbella noted, "If we had this information, we could start to draw connections to specific SEI structures and properties that lead to high-performance batteries."

## Insights from the new study

The *Joule* study distills recent research, much of which the Marbella group has led or contributed to, to present a case to leverage nuclear magnetic resonance (NMR) spectroscopy methods to connect the structure of the passivation layer on lithium to its actual function in the battery.

NMR enables researchers to directly probe how fast lithium ions move at the interface between the lithium metal anode and its passivation layer, while also providing a readout of the chemical compounds that are present on that surface.

While other characterization methods, like electron microscopy, may provide striking images of the SEI layer on the surface of lithium metal, they cannot pinpoint the exact chemical composition of disordered species, nor can they "see" ion transport. Other techniques that can probe lithium transport across the interface, like electrochemical analyses, do not provide chemical information.

Examining the data collected in Marbella's laboratory over the past six years, the team has found that NMR can uniquely sense changes in the structure of compounds in the SEI on lithium metal, which is key to explaining some of its more elusive structure-property relationships.

The researchers believe that combining multiple techniques, like NMR, other spectroscopies, microscopy, computer simulations, and electrochemical methods, will be necessary to develop and advance the development of lithium metal batteries.

## Applying NMR methods unveils new insights

When researchers expose lithium metal to different electrolytes, they often observe different performance metrics. Marbella's NMR experiment shows that these changes in performance arise because different electrolyte compositions create distinct SEI compositions and deliver lithium ions to the anode surface at different rates.

Specifically, when lithium metal battery performance improves, the rate of lithium exchange with the surface increases. They can now also see how the passivation layer should be arranged. To achieve the best performance, different chemical compounds must be layered on top of one another in the SEI, rather than randomly distributed.

The exchange experiments demonstrated in the new study can be used by materials scientists to help screen electrolyte formulations for high-performance lithium metal batteries as well as identify the surface compounds in the SEI that are required for high performance. Marbella adds that NMR is one of the only techniques—if not the only—that can probe the local structural changes of compounds in the SEI to address how ionically insulating materials may enable fast lithium-ion transport in the SEI.

"Once we know what structural changes are occurring—for instance, are things like lithium fluoride becoming amorphous, defected, nano-sized—then we can intentionally engineer these in and design lithium metal batteries that meet the performance metrics required for commercialization. The NMR experiment is one of the few that can accomplish this task and give us the very information essential to pushing anode surface design forward."

Marbella's group is currently using exchange NMR coupled with electrochemistry to provide a deeper understanding of SEI composition and properties in different electrolytes for lithium metal batteries. They are also developing systems that can determine individual chemical components' role in lithium-ion transport through the SEI.

**More information:** Using NMR spectroscopy to link structure to function at the Li solid electrolyte interphase, *Joule* (2024). DOI: 10.1016/j.joule.2024.04.016.
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