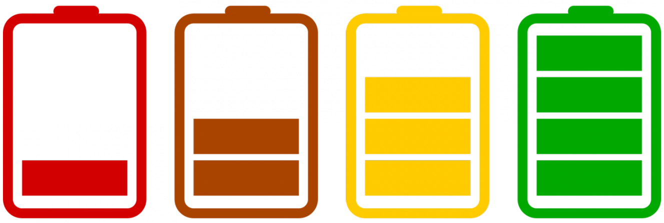
New design strategy for longer lasting batteries

23 January 2017, by Amanda Morris



Credit: CC0 Public Domain

It's always exciting to bring home a new smartphone that seems to do anything, but it can be all downhill from there. With every charge and discharge cycle, the device's battery capacity lowers a little bit more—eventually rendering the device completely useless.

"Why does this degradation occur? In some cases, we know; in other cases, we don't," said Northwestern Engineering's Christopher Wolverton. "But, in many cases, something probably happened to the cathode."

Wolverton, professor of materials science and engineering in Northwestern's McCormick School of Engineering, has developed a new computational design strategy that can pinpoint optimal materials with which to coat the cathode in lithium-ion batteries, protecting it from degradation and ultimately extending the battery's—and device's—life.

The cathode, which holds the battery's lithium ions when it is discharged, is typically a compound containing lithium, a transition metal, and oxygen. Batteries also contain an electrolyte, which is a transport medium for the lithium ions as they move between the cathode and the anode, which holds the lithium when the battery is charged. When the electrolyte decomposes, it can release hydrofluoric acid, a highly reactive substance that can attack the cathode. Researchers hypothesize this could be one reason why the battery loses capacity over time.

"A coating could serve multiple functions: it could provide a barrier around the cathode, preventing attack from hydrofluoric acid," Wolverton said. "Or a coating could preferentially react with the hydrofluoric acid, so there's none left to react with the cathode."

Partially supported by The Dow Chemical Company and US Department of Energy, Wolverton's design strategy and results were described in a recent issue of *Nature Communications*. Muratahan Aykol, a former graduate student in Wolverton's laboratory, was the paper's first author.

Wolverton previously developed the ever-growing Open Quantum Materials Database (OQMD), which was essential during his group's quest to find cathode coating materials. With information on more than 470,000 compounds, the OQMD is one of the world's largest materials databases, is open to the public, and can be downloaded online. Wolverton's group designed a way to screen through the database's materials that could be potential barriers to or scavengers of hydrofluoric acid. The group ultimately identified and ranked 30 top candidates, one of which the Dow Chemical Company has experimentally tested to discover that the coating did successfully prevent battery degradation.

"Having a massive database at hand allowed us to find the products of very complex, previously unexplored chemical reactions that determine the coating's effectiveness," said Aykol, who is now a postdoctoral fellow at Lawrence Berkeley National Laboratory. "Not only can we unveil a list of promising functional coatings, but we are helping our experimental colleagues target their resources to the best candidates."

While searching for cathode coatings is not a new venture, it has been an historically clumsy one. Researchers currently explore potential coating materials largely through trial-and-error, which can be a slow and limited process. Exploring every material and combination of materials can result in millions, or even billions, of possibilities—far too many to test experimentally.

"There has never really been a design strategy for these coating materials," Wolverton said. "Computationally, we can quickly screen the vast landscape of possible material combinations to pinpoint 25 compounds that are potentially very promising. Now, 25 is a more manageable number that you could test experimentally."

Wolverton said this design strategy extends beyond developing better batteries. It also aims to fulfill the vision of the Materials Genome Initiative, established by President Barack Obama in 2011 to help accelerate the discovery, development, and deployment of new materials.

"These kinds of databases and computational approaches, in principle, are not limited to batteries," Wolverton said. "We are using computation to help design many types of materials."

More information: Muratahan Aykol et al, High-throughput computational design of cathode coatings for Li-ion batteries, *Nature Communications* (2016). DOI: 10.1038/ncomms13779

Provided by Northwestern University
APA citation: New design strategy for longer lasting batteries (2017, January 23) retrieved 20 October 2019 from https://techxplore.com/news/2017-01-strategy-longer-batteries.html