A systematic way to find battery materials

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Lithium-ion batteries have become a leading energy source for everything from smartphones and laptops to power tools and electric cars, and researchers around the world are actively seeking ways to nudge their performance toward ever-higher levels. Now, a new analysis by researchers at MIT and the University of California at Los Angeles (UCLA) has revealed why one widely used compound works particularly well as the material for one of these batteries' two electrodes -- an understanding they say could greatly facilitate the process of searching for even better materials.

Lithium-ion batteries' energy and power density -- that is, how much electricity they can store for a given weight, and how fast they can deliver that power -- are determined mostly by the material used for the cathode (the positive electrode). When such batteries are being used, lithium atoms are stored within the crystal structure of the cathode; when the battery is being recharged, lithium ions flow back out of it. Many different materials are currently used for these cathodes.

But one of those materials has been a bit of a mystery. Lithium iron phosphate ($LiFePO_4$) performs well as a cathode, but this performance has been hard to explain because unlike other cathode materials, lithium ion phosphate seemed to require a two-phase process to store lithium — something that should theoretically reduce its efficiency, but for some reason does not.

That anomaly has now been explained. A more detailed analysis showed that, in fact, the compound was following a single-phase process after

all, but doing so in an unusual way -- which might point the way to discovery of many other such compounds that had previously been overlooked. The new analysis was carried out by Gerbrand Ceder, the Richard P. Simmons (1953) Professor of Materials Science and Engineering at MIT, his graduate student Rahul Malik, and postdoc Fei Zhou of UCLA, and published in the journal *Nature Materials*.

According to accepted theory, lithium iron phosphate "should have been a low-rate" cathode material, Ceder says — meaning that it could produce electricity only at a very low current, suitable for use with very-low-power devices. Instead, "it has become one of the highest-rate materials in use," something that "always puzzled us," he says.

Most cathode materials are porous, absorbing lithium ions during charging like water going into a sponge. But it was thought that lithium iron phosphate required a two-phase process, first forming one compound, which then morphed into a final, stable compound. The extra step was expected to add complexity and reduce the reaction's speed.

But the new experiments, which were able to probe the activity of the material as it absorbed the lithium, found that even though the material ends up reaching an equilibrium where it has two separate phases, in operation it actually undergoes a single-phase process. "The way it actually absorbs lithium is not two-phase," Ceder says, "but it separates into two phases when it's done."

That makes it much more similar to conventional single-phase cathode materials than had been thought -- and means that it makes sense to look at a wide range of other candidate materials that had been ignored because they were also assumed to require a two-phase process. This analysis makes it possible to "understand better which of these two-phase materials will actually work," Ceder says, opening up thousands of new candidate materials to be studied. "Now we have a way of

evaluating which materials may have potential," Ceder says. "It broadens the possibilities."

Previously, he says, it had been known that "some two-phase materials do zilch, some do very well," but nobody knew why. Now it is likely that the ones that work well are actually using a single-phase reaction, as turns out to be the case with lithium iron phosphate. Ceder and his colleagues have been developing computer algorithms that incorporate a wide variety of known properties of materials so that large numbers of candidates can be screened quickly and efficiently to search for very specific combinations of properties needed for a particular application.

Understanding the dynamics of how lithium ions get incorporated into different molecular structures "was the missing piece in the high-throughput screening process," Ceder says. "Hopefully we'll be able to do that better now."

Brent Fultz, professor of materials science and applied physics at the California Institute of Technology, who was not involved in this work, says these findings represent a "significant" step forward in understanding the behavior of this material.

"Some oddities in the crystal structure" of lithium iron phosphate have been known, he says, "including a solid solution phase that exists at temperatures only a bit above room temperature. What is so interesting about the work from this MIT group is that it shows how the solid solution phase is far from simple." He says "the authors make a strong case that the solid solution phase plays a bigger role in the performance" of this material than had been expected, and adds that "the work suggests alternative directions to the design of cathode materials for lithium batteries."

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