Method to predict the atomic structure of sodium-ion batteries

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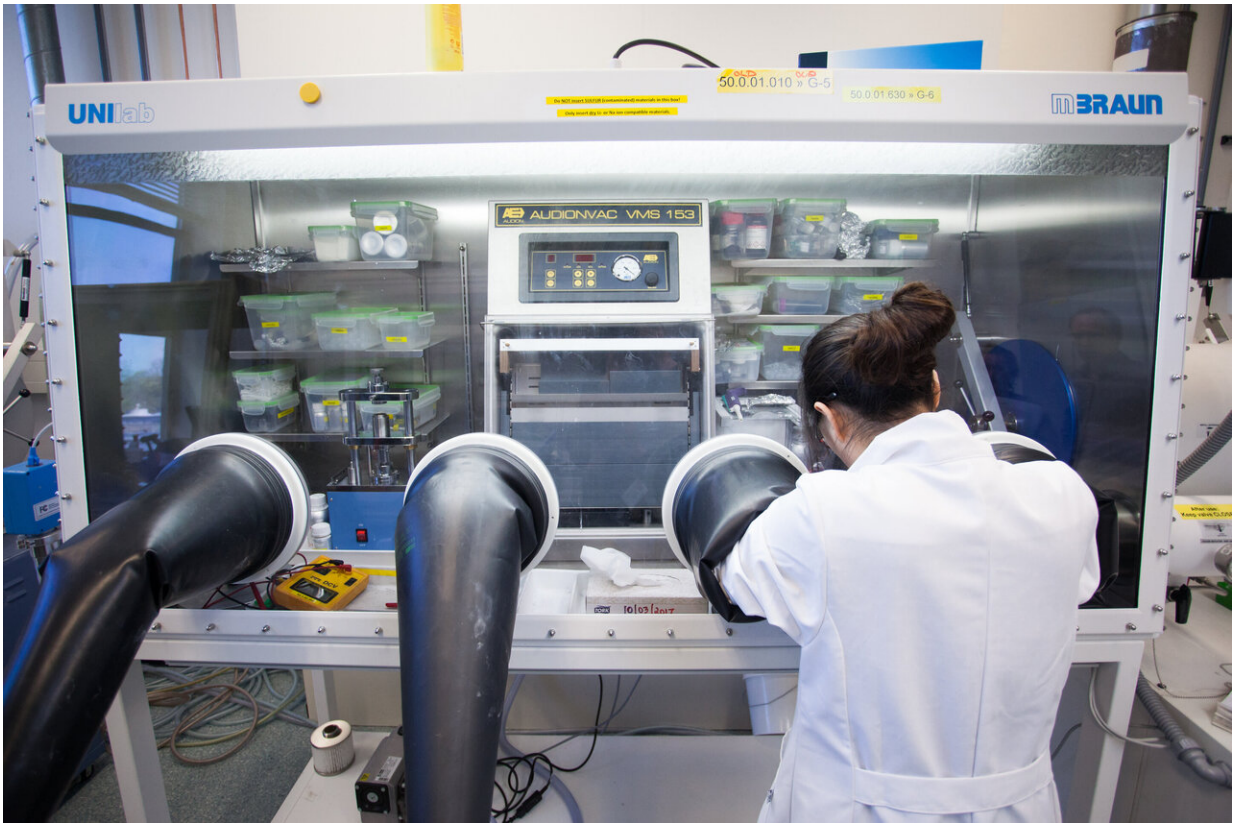


Credit: TU Delft

Researchers from the Chinese Academy of Sciences and Delft University of Technology (TU Delft) have developed a method to predict the atomic structure of sodium-ion batteries. Until now, this was

impossible even with the best supercomputers. The findings can significantly speed up research into sodium-ion batteries. As a result, this type of battery can become a serious technology next to the popular Li-ion batteries found in our smartphones, laptops and electric cars. The researchers have published their findings in the journal *Science*.

Mobile phones, laptops and electric cars all contain lithium-ion batteries. In terms of performance and energy density, these batteries are unrivaled. Yet the commercial dependence on one type of battery also has its disadvantages. Take cobalt, for example. So far, despite a great deal of research, producing lithium-ion batteries without this rare resource has not been possible. Cobalt is almost exclusively mined in Congo under harsh conditions and with a major impact on the environment.

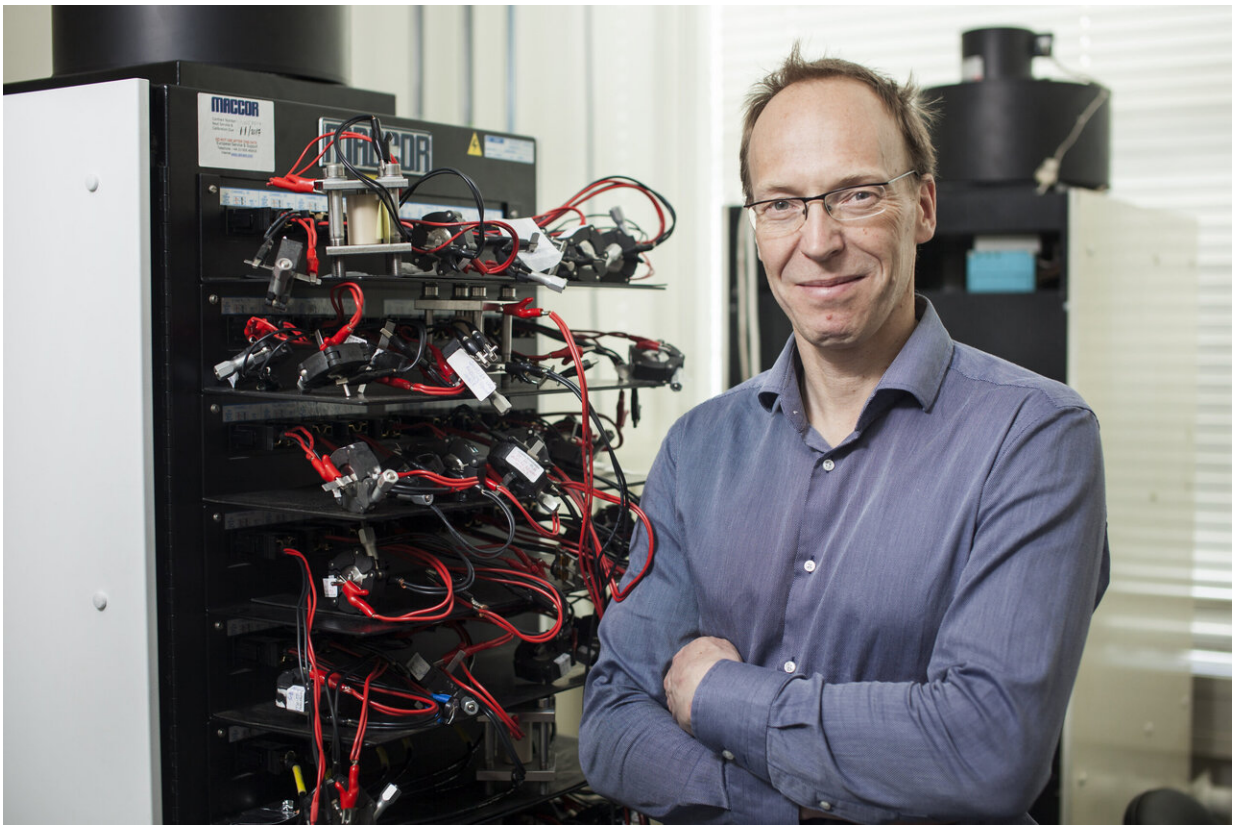
Lithium is a resource that can become problematic in the long run. "At the moment, we have more than enough of it," says TU Delft researcher Marnix Wagemaker. "But if we are all going to drive electrically in the future and if we need large batteries for storing solar energy at home, we will also need an enormous amount of lithium." That could become a problem because lithium reserves are anything but infinite.

Kitchen salt

Researchers believe sodium-ion batteries have potential. The name says it all: Instead of lithium, this type of battery is based on sodium, which is found in kitchen salt, among other things. In theory, Na-ion batteries do not perform as well as Li-ion batteries, but the gap is not that big. Wagemaker says, "At lab scale, Na-ion batteries can reach an energy density that is only 20 to 30% lower than that of Li-ion batteries. So they are not competitive when it comes to mobile phones or electric cars. But for situations in which weight is slightly less important, for example in maritime applications or in vehicles that can be charged frequently, they

can be a good alternative."

Na-ion batteries would also be suitable for stationary use, for example, in a power wall at home or in a battery park that stores wind and solar energy. In addition, Na-ion batteries provide more opportunities in the use of raw materials to build up better and cheaper positive electrodes. This versatility makes it much easier to get rid of cobalt, for instance, compared to the positive electrodes in Li-ion batteries. Cobalt is not only expensive but also poses an ethical problem from a standpoint of labor exploitation.



Credit: TU Delft

Infinite

Ironically, this versatility is also the sodium-ion battery's curse. Li-ion batteries only work with a limited number of raw materials and material structures, and it is relatively clear what the best 'recipe' for a cathode is. Not so for Na-ion batteries. "Depending on the precise cocktail of elements, you will end up with subtle differences in the atomic structure of the positive electrode, which have a major impact on the battery's performance," Wagemaker explains. "With just a handful of elements, there are so many structural possibilities that even the fastest supercomputer can't predict how the different combinations will turn out. As a result, the development of new materials is slow."

At least, that has been the case up to now. But the Delft researchers and their Chinese colleagues have found a way to predict the ideal recipe for the cathode. At an atomic level, a cathode looks much like a sandwich: it is made up of several layers, with ions in between. "At first it seemed like the size of the ions determined the atomic structure," says Wagemaker. "But it soon became clear that that wasn't the only factor. The distribution of the electrical charge of the ions plays a pivotal role."

Geology

This was a crucial insight for the researchers because the ratio between the size of an ion and its charge, the so-called "ionic potential," is known to have predictive value. "In geology, this relationship has been used for decades to understand why, for instance, certain iron oxides are more soluble than others," says Wagemaker. "This can reveal something about the formation of certain strata of the earth, or about other geological processes."

The question was whether this relationship would also be useful on an atomic scale. It turned out that it was. The researchers developed a

simple formula based on the ionic potential. "Using this formula we can predict which structure we will get at which ratio of a selection of raw materials," says Wagemaker. "The formula guides us through the enormous number of possibilities to the electrode materials that can deliver the best performance."

On the rise

The researchers also tested their formula by designing new materials. "We tried to make a cathode with the highest possible energy density, and one that you can charge very quickly," says Wagemaker. "In both cases, we succeeded. In terms of energy density we were right at the upper limit of what is possible. I like the fact that such a simple formula, based on a very old idea from geology, can make predictions on the atomic scale with such accuracy."

This research focused on one part of a battery: the cathode. A logical next step is to also look at other types of structures, both in electrodes and electrolytes for various types of batteries. Can this new approach also play a role there? Marnix Wagemaker thinks so. "We are going to explore that in the coming period. With this research we hope to speed up the development of materials for next generations of batteries."

More information: Zhao et al., Rational design of layered oxide materials for sodium-ion batteries. *Science* (2020), DOI: 10.1126/science.aay9972

Provided by Delft University of Technology

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