New framework from boron and silicon could smooth the way to higher capacities for lithium-ion batteries

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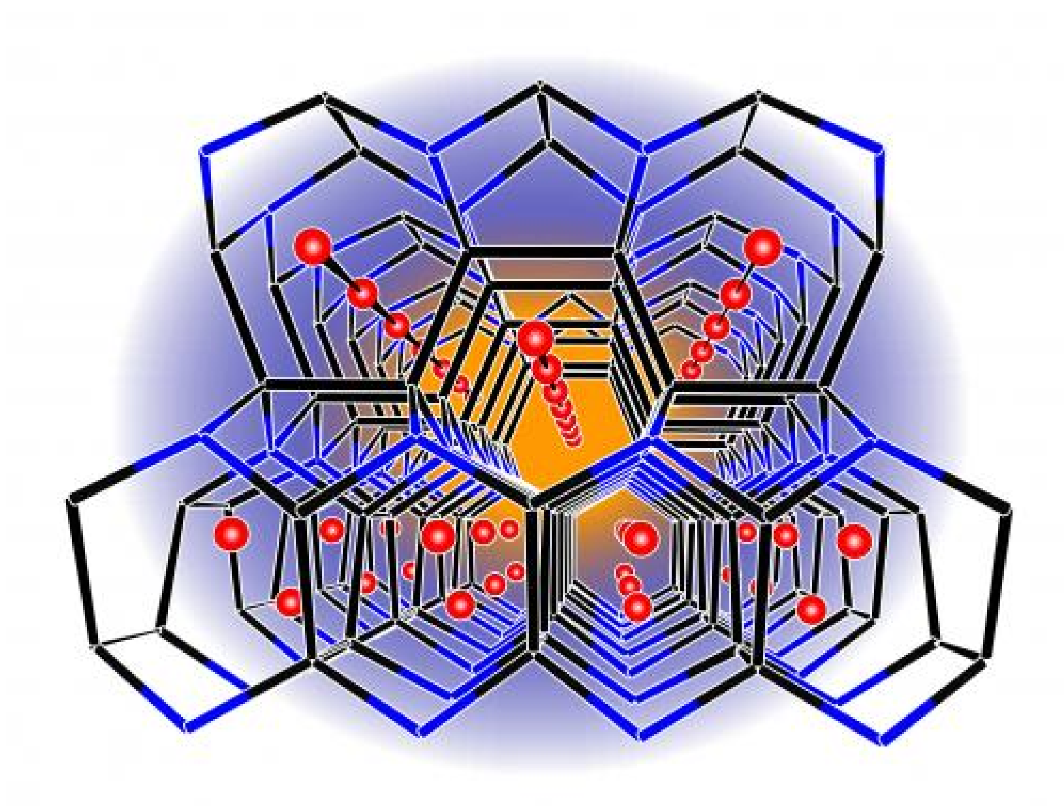

A newly synthesized borosilicid framework hosts lithium atoms in its channels, making it a promising candidate for electrodes of lithium-ion batteries. Credit: T. Faessler/M. Zeilinger, Technische Universitaet Muenchen

Laptops could work longer and electric cars could drive farther if it were possible to further increase the capacity of their lithium-ion batteries. The electrode material has a decisive influence on a battery's capacity. So far, the negative electrode typically consists of graphite, whose layers can store lithium atoms. Scientists at the Technische Universitaet Muenchen (TUM) have now developed a material made of boron and silicon that could smooth the way to systems with higher capacities.

Loading a lithium-ion battery produces lithium atoms that are taken up by the graphite layers of the negative electrode. However, the capacity of graphite is limited to one lithium atom per six carbon atoms. Silicon could take up to ten times more lithium. But unfortunately, it strongly expands during this process – which leads to unsolved problems in battery applications.

Looking for an alternative to pure silicon, scientists at the Technische Universitaet Muenchen have now synthesized a novel framework structure consisting of boron and silicon, which could serve as an electrode material. Similar to the carbon atoms in diamond, the boron and silicon atoms in the novel lithium borosilicide ($LiBSi_2$) are interconnected tetrahedrally. But unlike diamond they moreover form channels.

"Open structures with channels offer in principle the possibility to store and release lithium atoms," says Thomas Faessler, professor at the Institute of Inorganic Chemistry, Technische Universitaet Muenchen. "This is an important requirement for the application as anode material for lithium-ion batteries."

High-pressure synthesis

In the high-pressure laboratory of the Department of Chemistry and Biochemistry at Arizona State University, the scientists brought the starting materials lithium boride and silicon to reaction. At a pressure of

100,000 atmospheres and temperatures around 900 degrees Celsius, the desired lithium silicide formed. "Intuition and extended experimental experience is necessary to find out the proper ratio of starting materials as well as the correct parameters," says Thomas Faessler.

Lithium borosilicide is stable to air and moisture and withstands temperatures up to 800° Celsius. Next, Thomas Fässler and his graduate student Michael Zeilinger want to examine more closely how many lithium atoms the material can take up and whether it expands during charging. Because of its crystal structure the material is expected to be very hard, which would make it attractive as a diamond substitute as well.

Since the framework structure of lithium borosilicide is unique, Faessler and Zeilinger could give a name to their new framework. In honor of their university, they chose the name "tum."

More information: Michael Zeilinger, Leo van Wüllen, Daryn Benson, Verina F. Kranak, Sumit Konar, Thomas F. Fässler, and Ulrich Häussermann, LiBSi2: A Tetrahedral Semiconductor Framework from Boron and Silicon Atoms Bearing Lithium Atoms in the Channels, *Angewandte Chemie International Edition* 2013, 52, 5978-5982. DOI:10.1002/anie.201301540

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