Piling on pressure solves enduring mystery about metal's makeup

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Scientists have solved a decades-old puzzle about a widely used metal, thanks to extreme pressure experiments and powerful supercomputing.

Their discovery reveals important fundamental aspects of the element lithium, the lightest and simplest metal in the periodic table. The material is commonly used in batteries for phones and computers.

A mystery of how the metal's atoms are arranged—which influences properties such as its strength, malleability and conductivity—has been solved by their research.

An international team sought to better understand lithium's structure by studying it at cold temperatures. In this low-energy state, the fundamental properties of materials can be accurately observed.

Until now, it was difficult for scientists to explain previous experimental results indicating that lithium had a complex structure. To understand the theory properly required exceptionally accurate calculations using advanced quantum mechanics.

Their latest calculations, using the ARCHER supercomputer at the University of Edinburgh, found that lithium's structure is not complex or disordered, as previous results had suggested. Instead, its atoms are arranged simply, like oranges in a box.

Scientists suggest that in previous experiments, rapid cooling led to

misleading results. To avoid those problems, they reached low-temperature conditions by placing samples of lithium under extreme pressure - up to 4,500 times that of Earth's atmosphere—by squeezing it between a pair of diamonds. They then cooled and depressurised the sample before examining it using a synchotron device, which uses X-ray beams to see atoms.

The study, from the Universities of Edinburgh and Utah, was published in *Science*.

Dr Miguel Martinez-Canales, of the University of Edinburgh's School of Physics and Astronomy, said "Our calculations needed an accuracy of one in 10 million, and would have taken over 40 years on a normal computer."

Professor Graeme Ackland, of the University of Edinburgh's School of Physics and Astronomy, said: "We were able to form a true picture of cold lithium by making it using high pressures. Rather than forming a complex structure, it has the simplest arrangement that there can be in nature."

More information: "Quantum and isotope effects in lithium metal" *Science* (2017). science.sciencemag.org/cgi/doi … 1126/science.aal4886

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