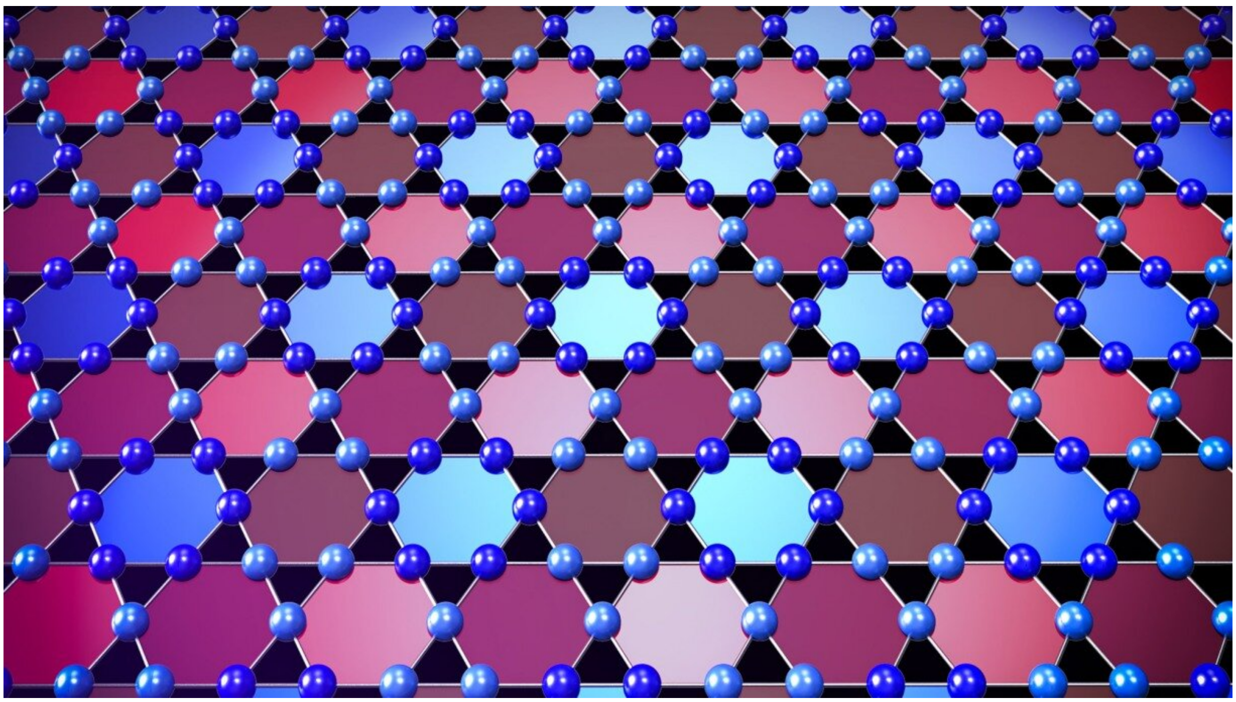
Researchers detail never-before-seen properties in a family of superconducting Kagome metals

February 10 2023



Brown researchers, working with an international team of scientists, describe the microscopic structure of Kagome superconductor RbV3Sb5 in a new study. Credit: M. Zahid Hasan and Jia-Xin Yin, Princeton University. Credit: Courtesy of the National Science Foundation multimedia gallery.

Dramatic advances in quantum computing, smartphones that only need to be charged once a month, trains that levitate and move at superfast speeds. Technological leaps like these could revolutionize society, but they remain largely out of reach as long as superconductivity—the flow of electricity without resistance or energy waste—isn't fully understood.

One of the major limitations for real-world applications of this technology is that the materials that make superconducting possible typically need to be at extremely cold temperatures to reach that level of electrical efficiency. To get around this limit, researchers need to build a clear picture of what different superconducting materials look like at the atomic scale as they transition through different states of matter to become superconductors.

Scholars in a Brown University lab, working with an international team of scientists, have moved a small step closer to cracking this mystery for a recently discovered family of superconducting Kagome metals. In a new study, they used an innovative new strategy combining nuclear magnetic resonance imaging and a quantum modeling theory to describe the microscopic structure of this superconductor at 103 degrees Kelvin, which is equivalent to about 275 degrees below 0 degrees Fahrenheit.

The researchers described the properties of this bizarre state of matter for what's believed to be the first time in *Physical Review Research*. Ultimately, the findings represent a new achievement in a steady march toward superconductors that operate at higher temperatures. Superconductors that can operate at room temperature (or close to it) are considered the holy grail of condensed-matter physics because of the tremendous technological opportunities they would open in power efficiency, including in electricity transmission, transportation and quantum computing.

"If you are ever going to engineer something and make it commercial, you need to know how to control it," said Brown physics professor

Vesna Mitrović, who leads a condensed matter NMR group at the University and is a co-author on the new study. "How do we describe it? How do we tweak it so that we get what we want? Well, the first step in that is you need to know what the states are microscopically. You need to start to build a complete picture of it."

The new study focuses on superconductor RbV3Sb5, which is made of the metals rubidium vanadium and antimony. The material earns its namesake because of its peculiar atomic structure, which resembles a basketweave pattern that features interconnected star-shaped triangles. Kagome materials fascinate researchers because of the insight they provide into quantum phenomena, bridging two of the most fundamental fields of physics—topological quantum physics and condensed matter physics.

Previous work from different groups established that this material goes through a cascade of different phase transitions when the temperature is lowered, forming different states of matter with different exotic properties. When this material is brought to 103 degrees Kelvin, the structure of lattice changes and the material exhibits what's known as a charge-density wave, where the electrical charge density jumps up and down. Understanding these jumps is important for the development of theories that describe the behavior of electrons in quantum materials like superconductors.

What hadn't been seen before in this type of Kagome metal was what the physical structure of this lattice and charge order looked like at the temperature the researchers were looking at, which is highest temperature state where the metal starts transitioning between different states of matter.

Using a new strategy combining NMR measurements and a modeling theory known as density functional theory that's used to simulate the electrical structure and position of atoms, the team was able to describe the new structure the lattice changes into and its charge-density wave.

They showed that the structure moves from a 2x2x1 pattern with a signature Star of David pattern to a 2x2x2 pattern. This happens because the Kagome lattice inverts in on itself when the temperature gets extremely frigid. The new lattice it transitions into is made up largely of separate hexagons and triangles, the researchers showed. They also showed how this pattern connects when they take one plane of the RbV3Sb5 structure and rotate it, "gazing " into it from a different angle.

"It's as if this one Kagome now becomes these complicated things that split in two," Mitrović said. "It stretches the lattice so that the Kagome becomes this combination of hexagons and triangles in one plane and then in the next plane over, after you rotate it half a circle, it repeats itself."

Probing this atomic structure is a necessary step to providing a complete portrait of the exotic states of matter this superconducting material transitions into, the researchers said. They believe the findings will lead to further prodding on whether this formation and its properties can help superconductivity or if it's something that should be suppressed to make better superconductors. The new unique technique they used will also allow the researchers to answer a whole new set of questions.

"We know what this is now and our next job is to figure out what is the relationship to other bizarre phases at low temperature—does it help, does it compete, can we control it, can we make it happen at higher temperatures, if it's useful?" Mitrović said. "Next, we keep lowering the temperature and learning more."

The experimental research was led by Jonathan Frassineti, a joint graduate student between Brown and the University of Bologna, Giuseppe Allodi from the University of Parma, and two Brown students: Erick Garcia and Rong Cong. Theoretical work was led by Pietro Bonfà while all the materials were synthesized at the University of California Santa Barbara. This research included funding from the National Science Foundation.

More information: Jonathan Frassineti et al, Microscopic nature of the charge-density wave in the kagome superconductor RbV_3Sb_5, *Physical Review Research* (2023). DOI: 10.1103/PhysRevResearch.5.L012017

Provided by Brown University