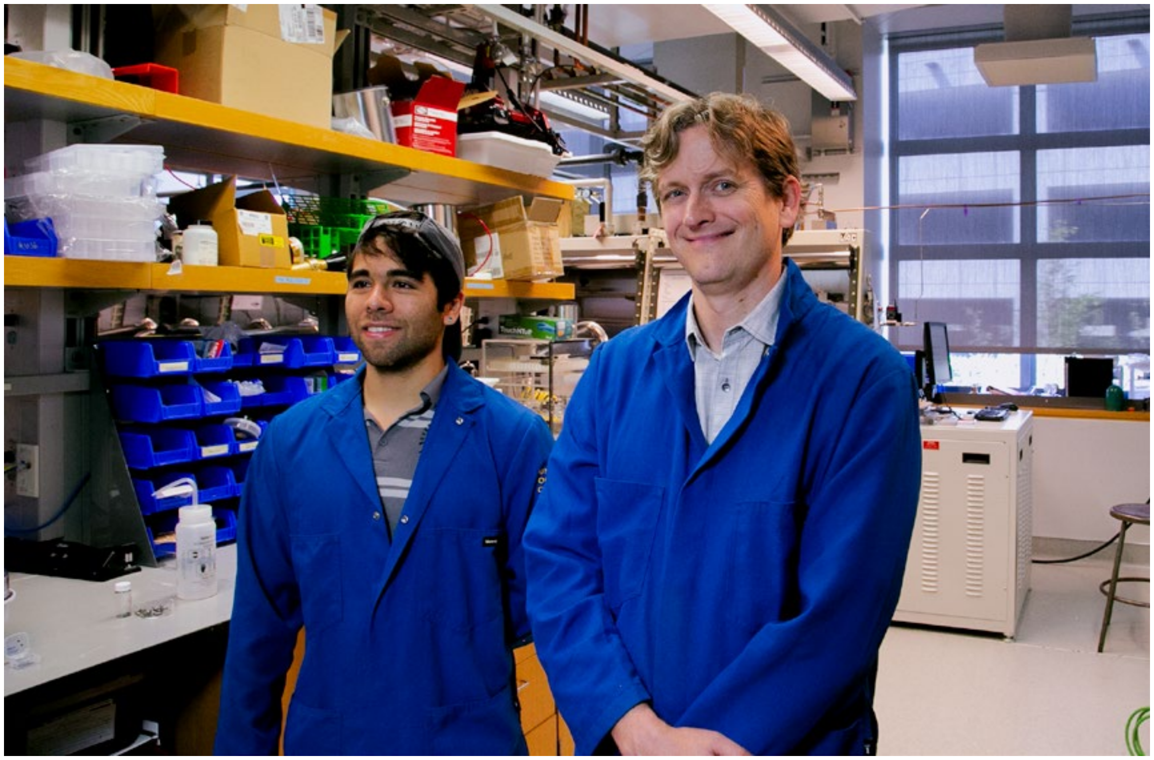
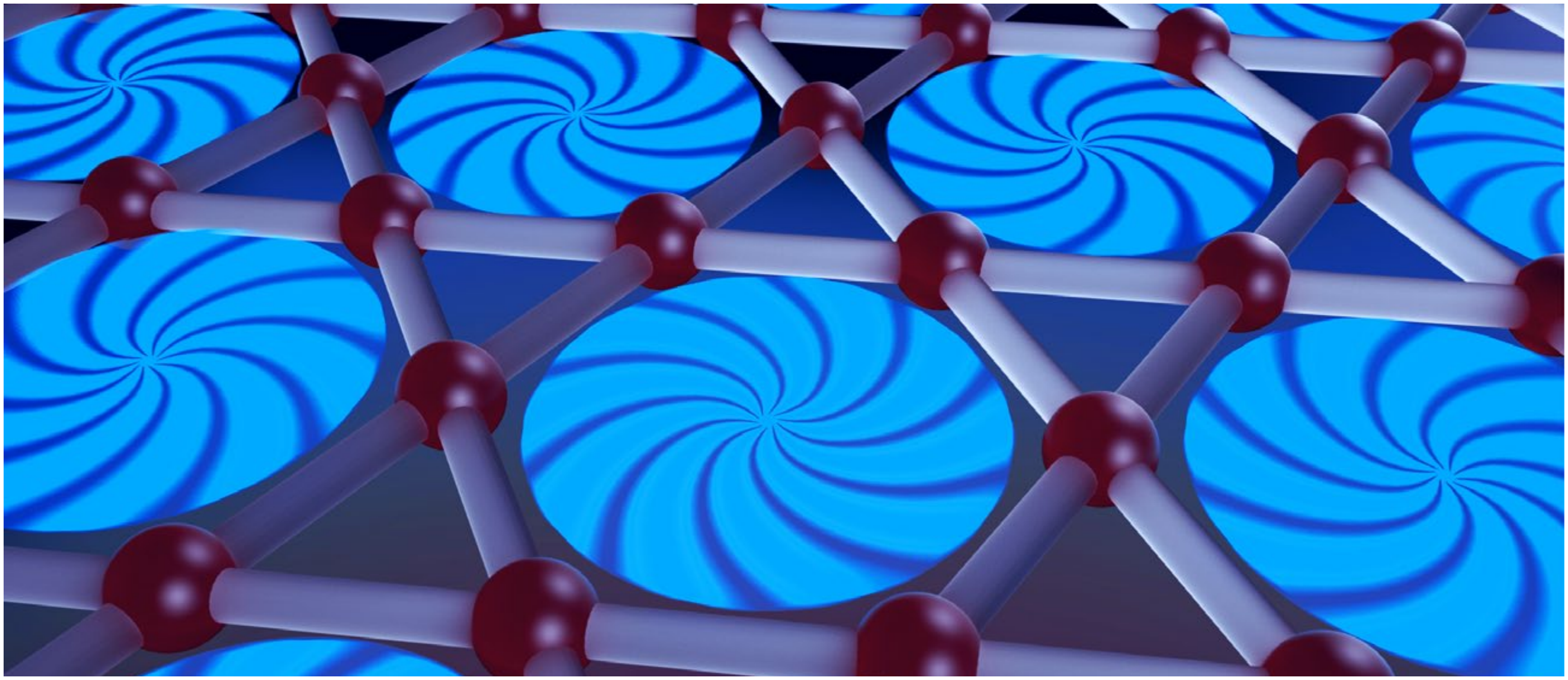


Stephen Wilson (right) and postdoctoral researcher Brenden R. Ortiz, who discovered the new material.

A NEW MATERIAL EXCITES RESEARCHERS AROUND THE WORLD

Created at UCSB's National Science Foundation Quantum Foundry, the material may be a unique kind of superconductor

Since receiving a $25 million grant in 2019 to become the first National Science Foundation (NSF) Quantum Foundry, UC Santa Barbara researchers affiliated with the Foundry, including co-director and materials professor **Stephen Wilson,** have been working to develop materials that can enable quantum information–based technologies for such applications as quantum computing, communications, sensing, and simulation.



Concept illustration shows what makes this superconductor special: its rare kagome lattice, formed by connected triangles in a two-dimensional array, making it a highly favorable testbed for physicists' theories of superconductivity. Illustration by Brian Long

In a new paper, published June 10, 2021 in the journal *Nature Materials*, Wilson and more than twenty co-authors, including key collaborators at Princeton University, describe a new material developed in the Quantum Foundry as a superconductor candidate — a material in which electrical resistance disappears and magnetic fields are expelled from the material — that could be useful in future quantum computation.

As a prelude, last year, a paper published by Wilson's group in the journal *Physical Review Letters* and featured in *Physics* magazine, described a new material, cesium vanadium antimonide (CsV_3Sb_5), that exhibits a surprising mixture of characteristics involving a self-organized patterning of charge intertwined with a superconducting state. The discovery was made by Elings Postdoctoral Fellow **Brenden R. Ortiz** and, as it turns out, Wilson says, those characteristics are shared by a number of related materials, including RbV_3Sb_5 and KV_3Sb_5, the latter (a mixture of potassium, vanadium, and antimony) being the subject of this most recent paper, titled "Discovery of unconventional chiral charge order in kagome superconductor KV_3Sb_5."

Materials in this group of compounds, Wilson notes, "are predicted to host interesting charge density wave physics [that is, their electrons self-organize into a non-uniform pattern across the metal sites in the compound]. The peculiar nature of this self-organized patterning of electrons is the focus of the current work."

This predicted charge density wave state and other exotic physics stem from the network of vanadium (V) ions inside these materials, which form a corner-sharing network of triangles known as a kagome lattice. KV_3Sb_5 was discovered to be a rare metal built from kagome lattice planes, one that also superconducts. Some of the material's other characteristics led researchers to speculate that charges in it may form tiny loops of current that create local magnetic fields.

> You can imagine the charge moving around in a little loop.... Such a state would be a new electronic state of matter and would have important consequences for the underlying unconventional superconductivity.

Materials scientists and physicists have long predicted that a material could be made that would exhibit a type of charge density wave order that breaks what is called *time reversal symmetry.* "That means that it has a magnetic moment, or a field, associated with it," Wilson says. "You can imagine that there are certain patterns on the kagome lattice where the charge is moving around in a little loop. That loop is like a current loop, and it will give you a magnetic field. Such a state would be a new electronic state of matter and would have important consequences for the underlying unconventional superconductivity."

The role of Wilson's group in the Foundry was to make the material and characterize its bulk properties. The Princeton team then used high-resolution scanning tunnelling microscopy (STM) to identify what they believe are the signatures of such a state, which, Wilson says "are also hypothesized to exist in other anomalous superconductors, such as those that superconduct at high temperature, though it has not been definitively shown."

STM works by scanning a very sharp metal wire tip over a surface. By bringing the tip extremely close to the surface and applying an electrical voltage to the tip or to the sample, the surface can be imaged down to the scale of resolving individual atoms and where the electrons group. In the paper, the researchers describe seeing and analyzing a pattern of order in the electronic charge, which changes as a magnetic field is applied. This coupling to an external magnetic field suggests a charge density wave state that creates its own magnetic field.

This is exactly the kind of work for which the Quantum Foundry was established. "The Foundry's contribution is important," Wilson says. "It has played a leading role in developing these materials, and Foundry researchers discovered superconductivity in them and then found signatures indicating that they may possess a charge density wave. Now, the materials are being studied worldwide, because they have various aspects that are of interest to many different communities."

Wilson explains further: "They are of interest, for instance, to people in quantum information as potential topological superconductors; they are of interest to people who study new physics in topological metals, because they potentially host interesting correlation effects, defined as the electrons' interacting with one another, and that is potentially what provides the genesis of this charge density wave state. And they're of interest to people who are pursuing high-temperature superconductivity, because they have elements that seem to link them to some of the features seen in those materials, even though KV_3Sb_5 superconducts at a fairly low temperature."

If KV_3Sb_5 turns out to be what it is suspected of being, it could possibly be used to make a topological qubit useful in quantum information applications. For instance, Wilson says, "In making a topological computer, one wants to make qubits whose performance is enhanced by the symmetries in the material, meaning that they don't tend to decohere [decoherence of fleeting entangled quantum states being a major obstacle in quantum computing] and therefore have a diminished need for conventional error correction.

"There are only certain kinds of states you can find that can serve as a topological qubit, and a topological superconductor is expected to host one," he adds. "Such materials are rare. This system may be of interest for that, but it's far from confirmed, and it's hard to confirm whether it is or not. There is a lot left to be done in understanding this new class of superconductors."

cooking up a SUPERCONDUCTOR

The making of a novel, new material

As a physics graduate student at the Colorado School of Mines (CSM), **Brenden R. Ortiz,** now a postdoctoral researcher in the lab of UC Santa Barbara materials professor **Stephen Wilson,** was looking for new materials related to energy efficiency. A mix of intuition and experience led him to believe that mixing the element antimony with the alkali metals on the Periodic Table was a promising way to proceed. Because most materials made from two elements had already been discovered, however, Ortiz decided he would need to combine at least three elements. "Solid-state chemistry is a bit like cooking," he says. "To find something novel, you have to be willing to experiment with new combinations and accept that some of your creations might be failures."

Ortiz eventually conducted numerous experiments, each a unique combination of antimony, one alkali metal, and one transition metal. He put small pieces of each element into a vial, which was shaken in a machine to yield a powder. He then pressed each powder into a small disc, heated it, polished it, and examined it with an electron microscope.

Ortiz deliberately made samples that were "impure" and contained swirls and pockets, like a marbled cake, indicating how and where the elements had mixed. "What you see is a spotted pattern, with regions of white, gray, and black," he says. "It's easy to visually identify the different regions of interest, and once you see them, you can use electron microscopy to identify the ratio of each element in the mixture."

By cross-referencing the elemental ratios extracted from electron microscopy with databases of known compounds, he was able to identify any new compounds he had made. He then had to identify the crystal structure. "At first, you know what the mate-

Brenden R. Ortiz, postdoctoral researcher in Stephen Wilson's materials lab at UCSB, separates newly grown crystals, the result of placing the mixed elements in a steel capsule, heating them to one thousand degrees Celsius, then slowly cooling them to five hundred degrees over a two-week period. Here, he begins the laborious task of using tweezers and solvent to separate the crystals from unwanted residue.

rial is made of, but you don't know how it's put together," he says.

It is possible to perform X-ray diffraction on the powder as a way to see the structure, but that process gives a kind of "fingerprint" of the structure, and, Ortiz says, "If you don't have any matching fingerprints [in a database], it doesn't help you. You still don't know how it's arranged."

Today's powerful computers, however, make it possible to reverse-engineer the fingerprint to provide the actual structure. By having the powders characterized at a national laboratory, he successfully solved the structure of several of the new materials. The crystal structure of one such combination, a mixture of alkali (A), vanadium (V) and antimony (Sb) — AV_3Sb_5 — comprised a distinctive arrangement of six-pointed stars and hexagons. He soon realized that the material was a new manifestation of a *kagome lattice,* which holds special significance for materials scientists and physicists, owing to the unique and varied properties arising from its unusual crystal geometry.

When cooled to temperatures near absolute zero, kagome lattices serve as an ideal testbed for theories related to the fundamentals of quantum mechanics. "The kagome lattice on its own, especially if it's a metal, imparts some special characteristics just by the very nature of the atoms being arranged in that pattern. If it's a kagome *metal,* you're guaranteed to have some weird physics" Ortiz says.

Realizing that the structure was unique and potentially interesting, Ortiz and his collaborators at CSM knew that they would need to grow single crystals of the materials. The data from the powders *implied* certain properties, but the definitive way to identify a structure or measure its properties begins with growing a single crystal. "If you can do that, a single-crystal X-ray diffractometer can then tell you exactly what it is, no questions asked," he says. "You essentially have a full picture of the crystal."

Ortiz describes the process as "essentially growing rock candy," although it did take him a year and a half to develop the specifics. "You dissolve sugar (the solute) in water (the solvent) and heat it as a solution. Then, you slowly cool it down or evaporate off some of the water, and over time the water can't hold as much sugar. The sugar starts to fall out, and you get the crystallized cubes of sugar. I do exactly the same thing; the only difference is that, in my case, I dissolve the cesium vanadium antimonide in a flux, a mixture of cesium and antimony."

He puts the mixture inside a miniature steel "bomb," heats it to a thousand degrees Celsius, and then cools it very slowly, about one degree per hour, down to five hundred degrees. After two weeks, he pulls it out, breaks it open, and gets what looks like a geode with the crystals scattered through it. He then uses liquid and tweezers to extract them.

Ortiz published his discovery in the journal *Physical Review of Materials,* although it initially generated limited interest, and other prestigious journals turned the manuscript down.

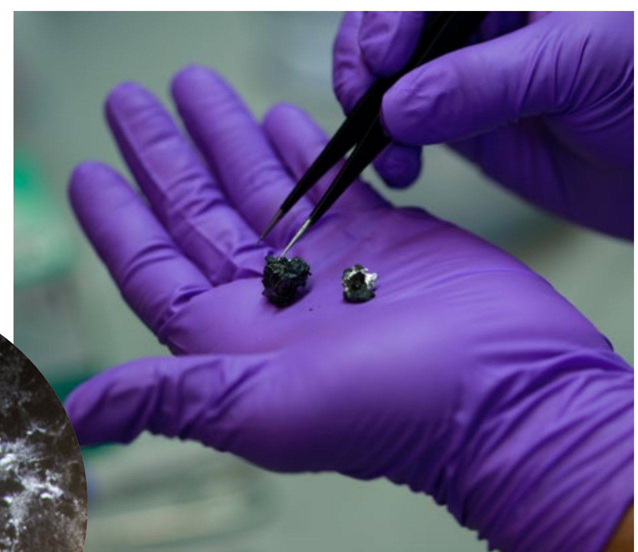
Six months later, he joined Wilson's lab as an Eilings Fellow and brought the new material with him, with the approval of Eric Toberer, his PhD advisor at CSM. Ortiz included a description of the material in his fellowship proposal, saying essentially that he had new kagome lattices but didn't know much about them, because CSM did not have the low-temperature equipment essential to inducing the material's most interesting idiosyncratic behavior.

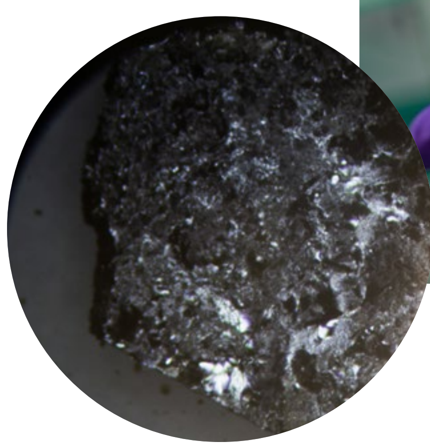
A couple of months after arriving at UCSB, Ortiz was thinking that he had done a lot of measurements on the KV_3Sb_5, the first material he had made, but not on the other two. Then, while performing a suite of measurements, he discovered to his surprise that the cesium compound (CsV_3Sb_5) superconducted. He recalls that, after confirming that superconductivity occurred throughout the crystal, Wilson said, "We need to send it to collaborators to get measurements going as we are publishing, because people go crazy for new superconductors."

The material was special in another way, too, as one of the few superconducting kagome lattices known to exist in the 2D state. The material is built up by having sheets of lattices stacked on top of each other. In 3D materials, the planes are linked, but in this material, Ortiz notes, "They are separate; they hardly talk to each other, making this a nearly 2D material, and many models and theories are easier to formulate and test in 2D than in 3D."

After no initial interest, the paper has generated a flurry of activity, with nearly one hundred citations since December 2020 and researchers all over the world asking Ortiz for crystals. He is currently growing them as fast as he can. "The theories that could result from this are intriguing," he notes, "in applications from fundamental science to quantum computing, which is why everyone is so interested in it.

"It's overwhelming how this has blown up," he adds. "The world is learning so quickly that I can no longer keep up with the narrative of my own discovery. It's like you have a kid and you have to let it grow up. The kid is out of my control now. He's out in the world, and he's got a jet. I'm honored when people ask for samples, and I'm ecstatic to collaborate. It's just an honor to have people say, 'We want *your* crystals of *your* material.'"





A superconductor in the palm of his hand: Brenden R. Ortiz (right) displays newly grown crystals (magnified below), that will be sent to researchers around the world for further investigation of their unique properties..