Physicists trap electrons in a 3D crystal for the first time

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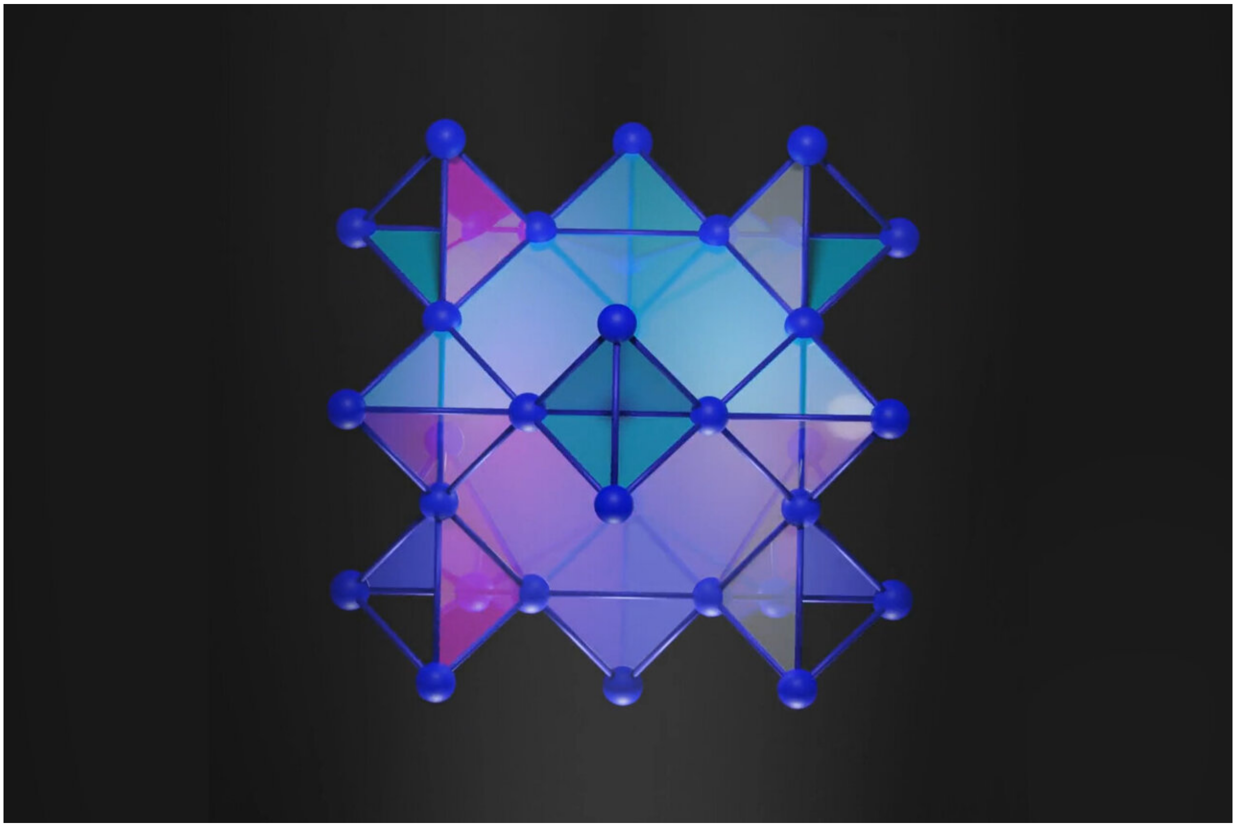

MIT physicists have trapped electrons in a pure crystal, marking the first achievement of an electronic flat band in a three-dimensional material. The rare electronic state is thanks to a special cubic arrangement of atoms (pictured) that resembles the Japanese art of “kagome.” The results provide a new way for scientists to explore rare electronic states in 3D materials. Credit: Joseph Checkelsky, Riccardo Comin, et al

Electrons move through a conducting material like commuters at the height of Manhattan rush hour. The charged particles may jostle and bump against each other, but for the most part, they're unconcerned with other electrons as they hurtle forward, each with their own energy.

But when a material's electrons are trapped together, they can settle into the same energy state and behave as one. In physics, this collective, zombie-like state is known as an electronic "flat band." Scientists predict that when electrons are in this state, they can start to feel the quantum effects of other electrons and act in coordinated, quantum ways. Then, exotic behavior such as superconductivity and unique forms of magnetism may emerge.

Now, physicists at MIT have successfully trapped electrons in a pure crystal. It is the first time scientists have achieved an electronic flat band in a three-dimensional material. With some chemical manipulation, the researchers also showed they could transform the crystal into a superconductor—a material that conducts electricity with zero resistance.

The crystal's atomic geometry makes the electrons' trapped state possible. The crystal, which the physicists synthesized, has an arrangement of atoms that resembles the woven patterns in "kagome," the Japanese art of basket weaving. In this specific geometry, the researchers found that electrons were "caged," rather than jumping between atoms and settled into the same energy band.

The researchers say that this flat-band state can be realized with virtually any combination of atoms—as long as they are arranged in this kagome-inspired 3D geometry. The results in *Nature* provide a new way for scientists to explore rare electronic states in three-dimensional materials. These materials might someday be optimized to enable ultra-efficient power lines, supercomputing quantum bits, and faster, smarter electronic devices.

"Now that we know we can make a flat band from this geometry, we have a big motivation to study other structures that might have other new physics that could be a platform for new technologies," says study author Joseph Checkelsky, associate professor of physics.

Setting a 3-D trap

In recent years, physicists have successfully trapped electrons and confirmed their electronic flat-band state in two-dimensional materials. However, scientists have found that electrons that are trapped in two dimensions can easily escape out of the third, making flat-band states difficult to maintain in 2D.

In their new study, Checkelsky, Comin, and their colleagues looked to realize flat bands in 3D materials, such that electrons would be trapped in all three dimensions and any exotic electronic states could be more stably maintained. They had an idea that kagome patterns might play a role.

In previous work, the team observed trapped electrons in a two-dimensional lattice of atoms that resembled some kagome designs. When the atoms were arranged in a pattern of interconnected, corner-sharing triangles, electrons were confined within the hexagonal space between triangles, rather than hopping across the lattice. But, like others, the researchers found that the electrons could escape up and out of the lattice, through the third dimension.

The team wondered: Could a 3D configuration of similar lattices work to box in the electrons? They looked for an answer in databases of material structures and came across a certain geometric configuration of atoms, classified generally as a pyrochlore—a type of mineral with a highly symmetric atomic geometry. The pychlore's 3D structure of atoms formed a repeating pattern of cubes, the face of each cube resembling a kagome-like lattice. They found that, in theory, this geometry could effectively trap electrons within each cube.

Rocky landings

To test this hypothesis, the researchers synthesized a pyrochlore crystal in the lab.

"It's not dissimilar to how nature makes crystals," Checkelsky explains. "We put certain elements together—in this case, calcium and nickel—melt them at very high temperatures, cool them down, and the atoms on their own will arrange into this crystalline, kagome-like configuration."

They then measured the energy of individual electrons in the crystal to see if they fell into the same flat band of energy. To do so, researchers typically carry out photoemission experiments, in which they shine a single photon of light onto a sample, that in turn kicks out a single electron. A detector can then precisely measure the energy of that individual electron.

Scientists have used photoemission to confirm flat-band states in various 2D materials. Because of their physically flat, two-dimensional nature, these materials are relatively straightforward to measure using standard laser light. But for 3D materials, the task is more challenging.

"For this experiment, you typically require a very flat surface," Comin explains. "But if you look at the surface of these 3D materials, they are like the Rocky Mountains, with a very corrugated landscape. Experiments on these materials are very challenging, and that is part of the reason no one has demonstrated that they host trapped electrons."

The team cleared this hurdle with angle-resolved photoemission spectroscopy (ARPES), an ultrafocused beam of light that is able to target specific locations across an uneven 3D surface and measure the individual electron energies at those locations.

"It's like landing a helicopter on very small pads, all across this rocky landscape," Comin says.

With ARPES, the team measured the energies of thousands of electrons across a synthesized crystal sample in about half an hour. They found that, overwhelmingly, the crystal's electrons exhibited the same energy, confirming the 3D material's flat-band state.

To see whether they could manipulate the coordinated electrons into some exotic electronic state, the researchers synthesized the same crystal geometry, this time with atoms of rhodium and ruthenium instead of nickel. On paper, the researchers calculated that this chemical swap should shift the electrons' flat band to zero energy—a state that automatically leads to superconductivity.

Indeed, they found that when they synthesized a new crystal with a slightly different combination of elements, in the same kagome-like 3D geometry, the crystal's electrons exhibited a flat band, this time at superconducting states.

"This presents a new paradigm to think about how to find new and interesting quantum materials," Comin says. "We showed that, with this special ingredient of this atomic arrangement that can trap electrons, we always find these flat bands. It's not just a lucky strike. From this point on, the challenge is to optimize to achieve the promise of flat-band materials, potentially to sustain superconductivity at higher temperatures."

More information: Joseph Checkelsky et al, Three-dimensional flat bands in pyrochlore metal $CaNi_2$, *Nature* (2023). DOI: 10.1038/s41586-023-06640-1.
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