Researchers find unexpected roadblock to conductivity in Mott insulators

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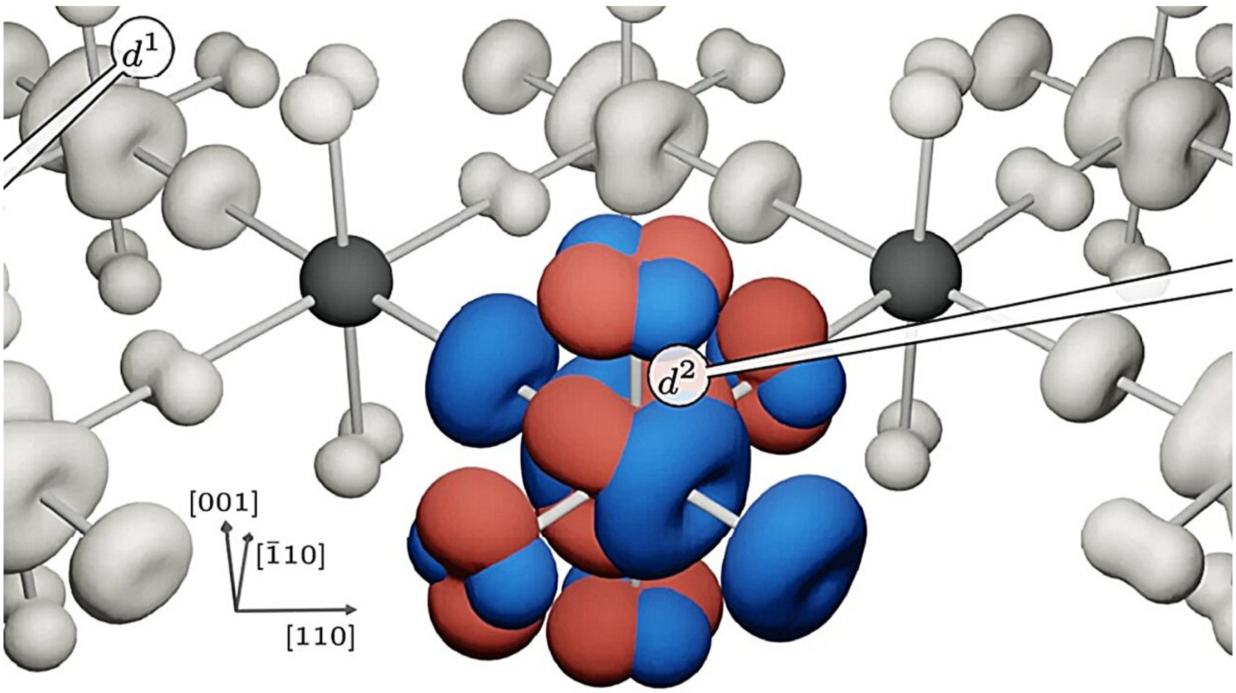

The researchers found the key to their theory is an unexpected collection of particles called bipolarons that form when electronic charge is added to the material. Credit: Mitrović Lab

In the realm of condensed matter physics, few phenomena captivate physicists' curiosity as much as Mott insulators. According to traditional theory, this odd class of materials should be capable of conducting electricity, yet they behave mostly as insulators.

What's even more bizarre is that when electrons are added, the material can actually become a superconductor, conducting an electric current with zero resistance. However, it can also stay an insulator no matter how many electrons are added. The extreme opposite reactions have puzzled scientists for decades, but some of those mysteries may be coming to an end.

Scientists from Brown University working with an international team of researchers have developed a novel theory, which they verified through a series of laboratory experiments, to fundamentally explain for the first time why one type of Mott insulator stubbornly resists conducting electricity even when electrons are added.

"It's the first time that we as physicists understand microscopically why the specific type of Mott insulator that we looked at has never been turned into a conductor," said Brown physics department chair and professor Vesna Mitrović, who leads a condensed matter magnetic resonance group at the University and is co-author on the new study.

"The work provides a really fundamental picture into why it may never work as a conductor. The main takeaway is the material is useful for other electronic applications, but not for turning into a conductor."

The work is described in *Nature Communications* and was done in collaboration with researchers from the University of Bologna, University of Vienna, University of Parma, Institute Polytechnique de Paris, Collège de France and the Ohio State University.

The work started as an unrelated condensed matter physics experiment between researchers from Brown and the University of Bologna.

The study focused on a type of Mott insulator called Ba_2Na_1–OsO_6. The material is what is known as a relativistic Mott insulator because it exhibits strong spin-orbit coupling, a state in which electrons both interact strongly with each other and their spin is greatly entangled with the way they move in their individual orbits.

Essentially, this makes the material deviate from more common physics predictions, which may create some special electronic behavior. Because of this, the material, and more generally the entire class of relativistic Mott insulators, has garnered considerable attention and investment by the scientific community to understand and control its properties.

Scientists think the material, like others in its class, can be moved in and out of the Mott insulating state by adding charge with electrons. The new study explains how previously unseen particles in this Mott insulator interact at the quantum level to stop it from turning into a conductor even when many extra electrons are added.

"This new understanding could save researchers a lot of time, investment and effort from trying different methods," Mitrović said.

The researchers found the key is an unexpected collection of particles called bipolarons that form when electronic charge is added to the material. Usually, the electrons spread out evenly in a metal, but here some of the charged electrons get stuck in certain spots of the material when added.

These trapped electrons are what comes together with the material's lattice structure to become bipolarons. The bipolarons then act like roadblocks for the electrons, making it hard for them to move around and conduct electricity.

Even when trying to overcome this roadblock by adding even more electrons, the bipolarons make sure the electrons keep getting stuck and are unable to move freely. Ultimately, this is what keeps the material an insulator.

This unexpected behavior puzzled the scientists because it goes against usual understanding of how materials respond to changes in their electronic structure. It's why results from the study took the researchers by surprise and the calculations for the theory took four years to put together, given that the interactions hadn't been studied before.

"According to our understanding of current physics, this shouldn't happen," Mitrović said.

The researchers now hope to put their new theory and experimentation techniques to the test and see how widespread bipolarons are in relativistic Mott insulators.

"It will be interesting to see if there are any circumstances that you can turn a relativistic Mott insulator into conductor or is this truly universal," Mitrović said.

More information: Lorenzo Celiberti et al, Spin-orbital Jahn-Teller bipolarons, *Nature Communications* (2024). DOI: 10.1038/s41467-024-46621-0

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