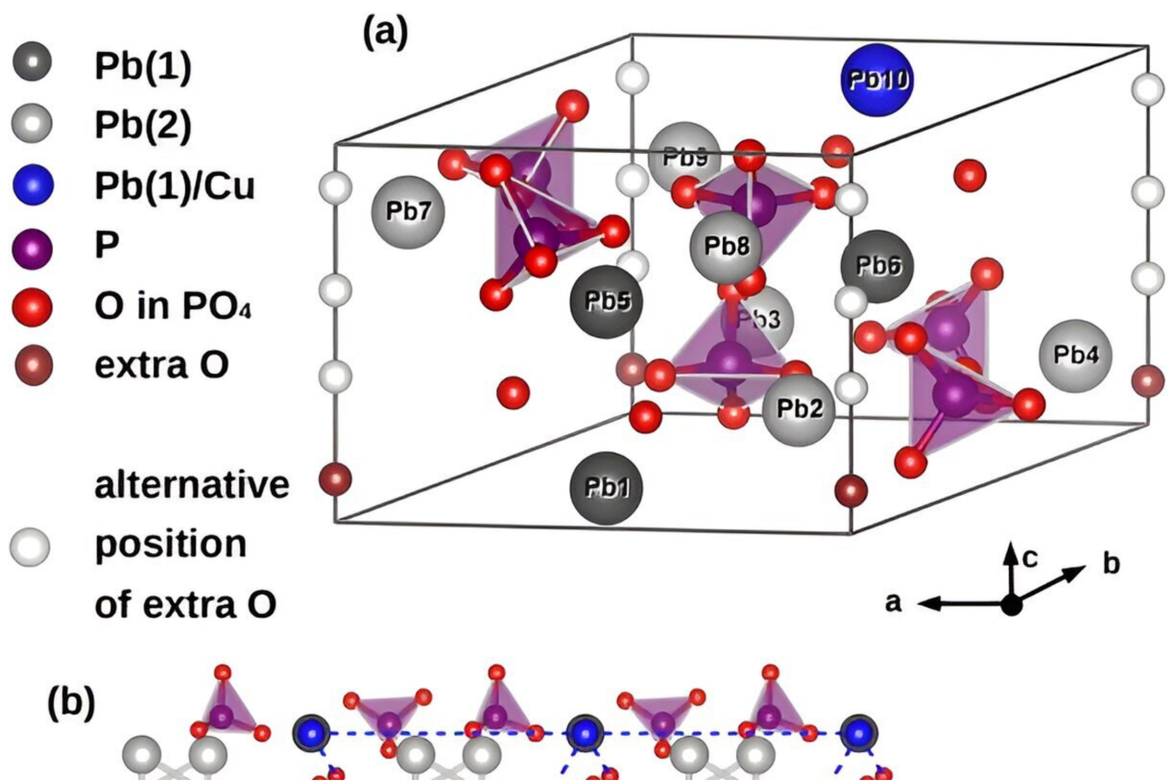
Newly discovered material has properties that could be advantageous for superconductivity

August 3 2023



Crystal structure of $Pb_9Cu(PO_4)_6O$: (a) single unit cell in side view; (b) four unit cells plus surrounding atoms in top view. There is some uncertainty regarding the position of the one extra O per formula unit and at which Pb site Cu is substituted. The extra O can occupy the dark red position as indicated in (a) or one of the empty white circles instead. As for the 10 Pb atoms in the unit cell, these fall into two symmetry classes: Pb(1) [dark gray] and Pb(2) [light gray]. The latter are located around the extra O, see (b). Our DFT calculations show that it is however energetically favorable for the Cu atom to be as far away from the extra O as possible, i.e., to occupy the blue Pb10 position of the Pb(2) class. This leaves us—for a lead-apatite structure and a single formula unit as unit cell—with the structure displayed. Credit: *arXiv* (2023). DOI: 10.48550/arxiv.2308.00676

LK-99 is the name of the material that is being hotly debated around the world these days: A Korean research group published results at the end of July 2023 on the preprint server *arXiv* suggesting that it could be a superconductor even at room temperature and normal atmospheric pressure. Superconductors known to date retain their properties only when either cooled to very low temperatures or subjected to extremely high pressure.

If this assumption is confirmed, it would be a huge breakthrough. Such a high-temperature superconductor has repeatedly been referred to as the "Holy Grail" of materials science. Such a material would revolutionize the way we generate, transport and store electricity and use electric motors. However, there are still justified doubts.

At TU Wien (Vienna), the material has now been analyzed with computer simulations and some interesting discoveries have been made: The calculated electron states are indeed quite favorable for superconductivity. Of course, this is not yet proof of superconductivity—but it is another reason to pay serious attention to the new material.

The first step is the band structure

Prof. Liang Si of Northwestern University Xi'an and Prof Karsten of the Institute of Solid State Physics at TU Wien started computer simulations to analyze the new material LK-99 immediately after the discovery became known. "The so-called band structure of the material is crucial," explains Karsten Held. "It tells us which combinations of velocity and energy are possible for the electrons in this material. If you know this band structure, you can tell a lot about the electrical properties of the material."

Using density functional theory, Liang Si and Karsten Held were able to calculate this band structure. It turns out that the electrical repulsion between the electrons means that the material in its pure form should actually be a so-called Mott insulator—a material that does not conduct any current at all, in a sense the opposite of a superconductor.

In the experiments, therefore, a doped version of the material was probably used unintentionally—i.e., one in which certain additional atoms were incorporated. And when extra electrons are added (or vice versa: removed) to the material by this kind of doping, the result looks completely different.

"We see relatively flat lines in the band structure, and we know that there are different mechanisms that can lead to superconductivity in such a band structure," says Held. So it does seem to be within the realm of possibility that LK-99 (with suitable doping) is a superconductor. "This is confirmed by another research group from Beijing, who concluded in initial experiments that LK-99 is a paramagnetic insulator. You have to dope the material to get the band structure that potentially enables superconductivity," Held said.

Three other research groups also performed density functional theory calculations at the same time with similar results. "This is not yet proof of high-temperature superconductivity; it is still possible that it is not a superconductor. But our results at least nourish the hope that it might indeed be a long-sought high-temperature superconductor," says Held.

Superconductivity or diamagnetism?

When a superconductor is placed on a magnet, electric current begins to flow on the surface of the superconductor, which in turn generates a magnetic field. The superconductor is repelled by the magnet and can thus float above the magnet. Therefore, one of the central arguments that LK-99 is a superconductor was a video showing LK-99 floating above a magnet. These experiments have since been confirmed by other experimental groups.

Criticism has been voiced, however, that this could be a different effect—there are, after all, various forms of magnetism. The best known is ferromagnetism, shown, for example, by pieces of iron that can be attracted with a magnet. Paramagnetic materials can also be attracted with a magnet, but unlike iron, they cannot be permanently magnetized themselves. The opposite of this is diamagnetism: diamagnetic materials are repelled by a magnet.

"Thus, it is conceivable that LK-99, if suspended above a magnet, could also be an ordinary diamagnet. This has also been repeatedly suspected in recent days," says Held. However, according to the theoretical calculations, he himself now considers this to be less likely.

"The electronic properties that we have calculated do not lead us to expect that LK-99 is a diamagnet. On the contrary, given the distribution of electrons, one would rather expect that LK-99 should be paramagnetic." The Beijing experiments show exactly that, a paramagnetic insulator. This would mean that levitation of the LK-99 samples would indeed indicate a transition to the superconducting state.

So has the "Holy Grail of materials science" now been found? Many more steps are needed to verify this. "There are still very good reasons to be skeptical," says Held. "I wouldn't bet my money at the moment that this is indeed a high-temperature superconductor—at least not at 1:1 betting odds. But the results at least show that LK-99 is indeed a very interesting material that deserves closer attention. It remains exciting."

More information: Liang Si et al, Electronic structure of the putative room-temperature superconductor $Pb_9Cu(PO_4)_6O$, *arXiv* (2023). DOI: 10.48550/arxiv.2308.00676

Provided by Vienna University of Technology