Optimizing electronic correlations for superconductivity

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(Phys.org) —The decadeslong effort to create practical superconductors moved a step forward with the discovery at Rice University that two distinctly different iron-based compounds share common mechanisms for moving electrons.

Samples from two classes of iron-based superconductors, pnictides and chalcogenides, employ similar coupling between electrons in their superconducting state, said Rice physicist Qimiao Si. Understanding that mechanism may help researchers find even better superconductors, he said.

The findings appear online today in a new *Nature Communications* paper by Si and colleagues in China and at Florida State University, George Mason University and the Los Alamos National Laboratory.

The pursuit of superconductivity—the ability of electrons to travel through a material with no resistance and producing no heat—has been a great challenge. But the rewards will be worth it, Si said, because superconductors will bring about revolutions not only in power generation and distribution, but also transportation, computing, medical imaging and more.

A superconductor has to be made of the right materials with electrons in just the right state. That depends on the temperature and how the materials' atoms – primarily the electrons – coordinate their activities. Experimental and theoretical analysis of the iron compounds helped the researchers define the delicate interplay of energies involved in the Mott transition (from metal to nonmetal), the superconducting transition temperature and the electron spin responsible for magnetism, which plays a key role in the finding, Si said.

"Historically, magnetism has been considered detrimental to superconductivity," he said. "We think of magnets sticking to the fridge and superconductors as living in entirely different worlds. And, in fact, the conventional theory of solids treats these two phenomena completely differently.

"That reinforced the notion that the two decouple. But in iron pnictides and chalcogenides, as well as some other materials, magnetism often comes hand in hand with superconductivity. That led us to ask the question: In which regime of this electron coupling could one find optimized superconductivity?"

The work by Si and his team showed how the interactions between electron spins in the iron-based compounds drive superconductivity. This interaction is the strongest when the electronic system is close to the Mott transition, which Si described as the point at which electrons teeter on the edge of free movement or being stuck in place.

"Ironically, this regime of electron correlation produces poor electrical conduction above the superconducting transition temperature, so the optimized superconductivity arises out of a bad metal," said Rong Yu, a co-author of the paper who was a postdoctoral fellow at Rice until this summer, when he became an associate professor at Renmin University in Beijing.

Part of the success of the work is to explain how superconductivity peaks of the two doped iron compounds have comparable transition temperatures, as has been observed experimentally.

"The chalcogenides, in many regards, are different from the pnictides but have a superconductive transition temperature just as high. That was a major surprise in the field," Si said.

Superconductors have to be kept cold. The compounds' superconducting properties activate at their transition temperatures, the points at which materials go from one phase to another – say, from a gas to a liquid or a liquid to a solid, as in steam to water to ice. Liquid helium-cooled superconductors have transition temperatures of about 4 degrees Kelvin. (That's -452 degrees Fahrenheit.) And what scientists consider "high-temperature" superconductors operate in conditions that would still frost a wampa.

While the long-term goal is to create superconductors that operate at room temperature, a good immediate target is 77 kelvins (-321 F), the boiling point of liquid nitrogen. Copper-based superconductors known as cuprates have achieved this goal, Si said, and the iron-based compounds he studies are closing in. "The record (for iron-based materials) is 56 K, but there's a sense in the community that we're not that far away," he said.

High temperature superconductivity was discovered in 2008 in the pnictides, irons doped with elements from Group 15 of the periodic table, including arsenic and phosphorus. The chalcogenides of interest to Si are even more recent creations. "This particular chalcogenide (a compound of potassium, iron and selenium) has only existed since late 2010," he said. "When it came out, we were surprised to see it has such a high transition temperature (a little above 30 K), given all the other electronic properties of this class of materials, which are very different from the pnictides."

More than two years ago, Si and his colleagues discovered that the "parent" members of the pnictides and chalcogenides occurred just on either side of the Mott transition. Their finding provided the understanding of the bad metallic behavior in both families of materials above their superconducting transition temperatures.

That work gave Si a head start to address the nature of superconductivity in both compounds. "In the present work, we conclude that the superconductive pairing of electrons is strongest near the Mott transition," he said.

The implications are great, Si said. Compared with the cuprates, the number of possible iron-based compounds is huge. Si and his colleagues think defining the underlying superconducting mechanism for irons will help researchers make materials that approach 77 K and, they hope, exceed it. That's important to industry, as liquid nitrogen drawn from air is far more abundant (and cheaper) than liquid helium.

More information: "Superconductivity at the border of electron localization and itinerancy." Rong Yu, Pallab Goswami, Qimiao Si, Predrag Nikolic, Jian-Xin Zhu. *Nature Communications* 4, Article number: 2783. DOI: 10.1038/ncomms3783. Published 15 November 2013

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