Study shows high-energy magnetic interactions alone don't cause high-temperature superconductivity

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From left: Researchers Giacomo Ghiringhelli, Chunjing Jia, Krzysztof Wohlfeld, Thomas Devereaux and Brian Moritz discuss the results of Jia's simulation. Credit: Fabricio Sousa/SLAC

(Phys.org) —A new theory and computer simulation by SLAC and Stanford researchers show that high-energy magnetic interactions are not the sole factor in making copper oxide materials perfect electrical conductors – superconductors – at relatively high temperatures.

This conclusion eliminates what many researchers had considered a primary pathway for finding new high-temperature superconductors. As a result, the mechanism for creating high-temperature superconductors remains as elusive as when the tantalizing phenomenon was discovered nearly 30 years ago, although the new result does narrow the search area.

"We'd all love to know how to make a room-temperature superconductor, which would save the world enormous amounts of energy," said Thomas Devereaux, leader of the research team and director of the Stanford Institute for Materials and Energy Sciences (SIMES), which is jointly run with SLAC. "But to do that we must understand what's happening inside the materials when they become superconducting. This result tells us that simply relating the high energy of magnetic interactions found in copper oxides with high temperature superconductivity is not the whole story."

The new theory and simulation were developed by Stanford graduate student Chunjing Jia and published recently in *Nature Communications*. Her calculations predict the atom-scale electronic and magnetic behavior of one of the most promising classes of high-temperature superconductors, copper oxides, as electrons are added or subtracted by a process called doping.

Jia ran the simulation on thousands of supercomputer processors at the National Energy Research Scientific Computing Center (NERSC). When she compared simulated changes in magnetic interactions over a wide range of doping conditions with the well-known rise and fall of superconductivity in copper oxides, they did not match.

"There was no correlation," Jia said. "If high-energy magnetic interactions were important in enabling high-temperature superconductivity in this material, we would have seen a rise and fall that matched its superconductivity."

Understanding High-Temperature Superconductors

Since the late 1950s, scientists have known how low-temperature superconductivity develops in certain metals and simple alloys within a few degrees of absolute zero: Electrons pair up and effortlessly ride waves of atomic vibrations that hold the pairs together like a virtual glue. According to that theory, the energy scale of the glue sets the maximum temperature at which the material is superconducting. Above that transition temperature, the glue fails as thermal vibrations increase; the electron pairs split up and superconductivity disappears.

In 1986, complex copper oxide materials were found to be superconducting at much higher – although still quite cold – temperatures. The discovery was so unexpected it caused a worldwide scientific sensation. Researchers speculated that superconductivity at room temperature might be possible if the mechanism that caused the new phenomenon could be found and optimized.

Until now, the most likely glue for holding electron pairs together at the higher superconducting temperatures seemed to be strong magnetic excitations created by interactions between electron spins. However, this study shows that those excitations are, at most, a minor factor.

Determining the precise details of the myriad interactions between the electrons in the complex copper oxide materials is exceedingly difficult. Fortunately, Jia's simulation also confirmed that a recently improved X-ray technique can help.

RIXS to the Rescue

The technique is called resonant inelastic X-ray scattering (RIXS). It involves illuminating a sample with X-rays that have just enough energy to excite some electrons deep inside the target atoms to jump up into a specific higher orbit. When the electrons relax back down into their previous positions, a tiny fraction of them emit X-rays that carry valuable atom-scale information about the material's electronic and magnetic configuration. When it was first demonstrated in the mid-1970s, however, the RIXS signal was too faint and blurry to be useful.

"You'd hit a material with 10 quadrillion X-ray photons and would be happy to get a few thousand in the detector," said Giacomo Ghiringhelli, associate professor of physics at the Polytechnic University of Milan in Italy. "It was very difficult to do significant research with so few photons."

That changed dramatically seven years ago when Ghiringhelli, Lucio Braicovich and other colleagues made a fundamental change to the RIXS technique that boosted its output by 100 to 1,000 times.

"Giacomo's and Lucio's innovation surprised everyone in the field," said Devereaux, who now collaborates with them. "RIXS suddenly became a big thing in X-ray spectroscopy."

As a result, new RIXS beamlines are being built at other X-ray light sources around the world. The Department of Energy recently approved a new RIXS experimental station for SLAC's Linac Coherent Light Source (LCLS), setting the stage for even more precise experiments at future high-repetition-rate X-ray free-electron lasers.

Moreover, Jia's simulation provided independent confirmation that RIXS is actually seeing the magnetic interactions.

"The fundamental insights we're gaining with RIXS and our theoretical simulations will ultimately help us learn how to design, from the atom up, new materials having specific and useful electronic and magnetic behaviors," Devereaux said. "Finding the conditions that enable high-temperature superconductivity is still at the top of our list."

More information: "Persistent spin excitations in doped antiferromagnets revealed by resonant inelastic light scattering." C. J. Jia et al, *Nature Communications* 5, 28 February 2014, DOI: 10.1038/ncomms4314

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