Modified nickelate materials could improve understanding of high-temperature superconductivity

March 13 2020

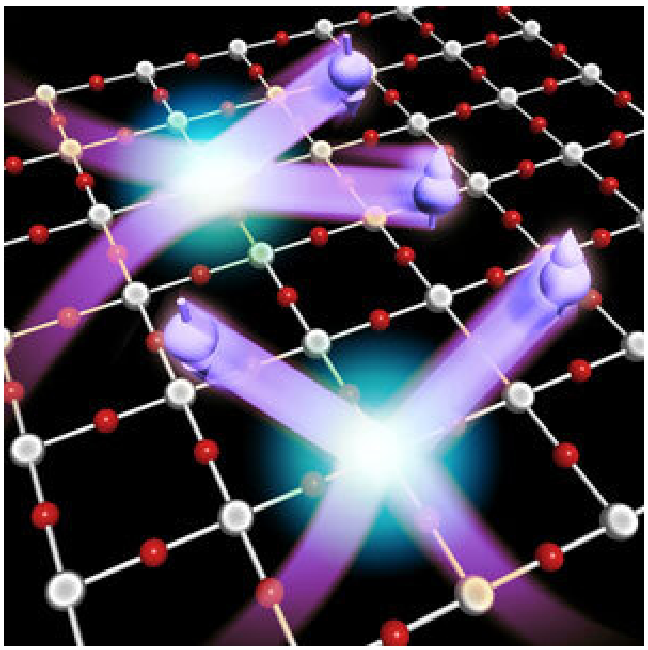

Figure 1: Electrons (lilac) interact strongly with one another as they move through the NiO2 layer of a nickelate material, which could act as a model for high-temperature superconductivity (nickel = gray, oxygen = red). (Image produced by Mari Ishida of the RIKEN Center for Emergent Matter Science.). Credit: RIKEN Center for Emergent Matter Science

The hunt for high-temperature superconductors could be aided by calculations by RIKEN physicists that have revealed the behavior of electrons in a nickel oxide material.

Superconductors can carry an electrical current with no resistance, and are used to make powerful electromagnets or sensitive instruments for measuring magnetic fields.

Conventional superconductivity depends on a form of electron pairing that occurs only at extremely low temperatures, so superconducting devices must be cooled with expensive liquefied gases. But about 30 years ago, researchers discovered that some cuprate materials could become superconductors at relatively warm temperatures, up to −140 degrees Celsius. The underlying cause of this high-temperature superconductivity is still not understood.

In 2019, researchers found that a strontium-doped neodymium nickel oxide ($Nd_{0.8}Sr_{0.2}NiO_2$) could superconduct below −258 degrees Celsius. The discovery attracted attention not because of the temperature, but because this nickelate material has a very similar crystal structure to the cuprates, and may serve as a test-bed to better understand how superconductivity works in these materials.

The nickelate material consists of alternating layers of Nd and NiO_2. Yusuke Nomura at the RIKEN Center for Emergent Matter Science and colleagues have now studied how the interactions between certain electrons in these two layers might influence superconductivity.

The team's calculations showed that the electrons in the NiO_2 layer strongly interact with each other, which is similar to cuprates where the strong correlation in the CuO_2 layer is believed to play a key role in their high-temperature superconductivity. However, there is a difference between the nickelates and the cuprates: in the nickelates, electrons in the neodymium layer are partially occupied and form the Fermi pocket, a relatively small region in the Brillouin zone surrounded by the Fermi surface. These pockets do not appear in cuprates, which may make the nickelate material an imperfect analogue for cuprates.

Nomura's team used computational models to study whether the pockets could be eliminated by tweaking the chemical composition of the material and hence create a nickelate that is a better match for the cuprates. They found that two compounds could fit the bill: sodium neodymium nickel oxide ($NaNd_2NiO_4$) and sodium calcium nickel oxide ($NaCa_2NiO_3$). "If the proposed nickelates are synthesized, they will be real nickel analogues of cuprate superconductors," Nomura notes.

"The next stage is to clarify the difference and similarity between the nickelates and cuprates in a more systematic way, and get deeper insight into the superconducting mechanism in both systems," he adds.

More information: Yusuke Nomura et al. Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor $NdNiO_2$, *Physical Review B* (2019). DOI: 10.1103/PhysRevB.100.205138

Provided by RIKEN