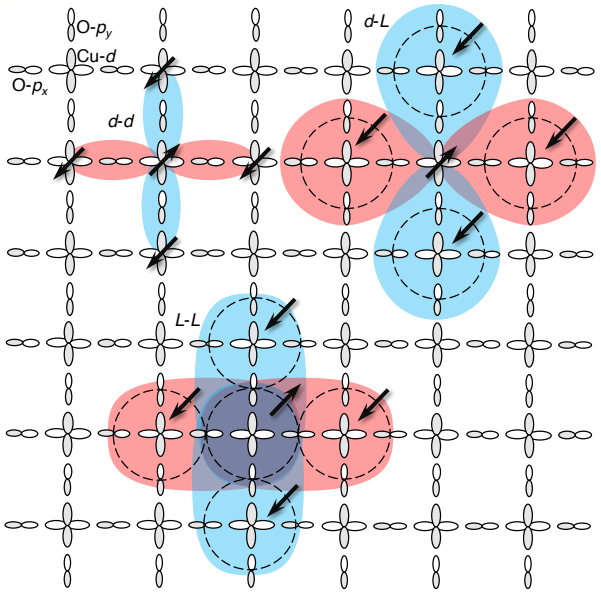
Advanced Simulations Reveal Orbital Structure of Cooper Pairs in High-Temperature Superconductors



Cu-d and O-$p_{x/y}$ orbitals in the CuO plane of the cuprate superconductors. Superconductivity arises from the formation of pairs with anti-parallel spins (↑,↓) composed of electron holes on the Cu-d and the bonding (L) combination of the four surrounding O-$p_{x/y}$ orbitals. All orbital components of the pairs have the same d-wave (+ (red) along x, - (blue) along y direction) structure, justifying a simpler single-band description.

P. Mai, G. Balduzzi, S. Johnston, T. A. Maier, Orbital structure of the effective pairing interaction in the high-temperature superconducting cuprates, *npj Quantum Materials* **6**, 26 (2021).

Scientific Achievement

Quantum Monte Carlo simulations reveal that Cooper pairs in the cuprate high-T_c superconductors are composed of electron holes on the Cu-*d* orbital and on the bonding molecular orbital constructed from the four surrounding O-*p* orbitals.

Significance and Impact

The results provide new information on the mechanism responsible for superconductivity in the cuprates and explain how an effective single-orbital Hubbard model successfully captures their properties.

Research Details

- Large-scale computations of a realistic three-band Hubbard model enabled, for the first time, a detailed study of the orbital structure of the cuprate pairing interaction
- The results provide strong support for the Zhang-Rice singlet framework, which constructs a quasiparticle that can effectively be described in terms of a simpler single-band model.

Work was performed at Oak Ridge National Laboratory.

U.S. DEPARTMENT OF ENERGY | Office of Science
SciDAC Scientific Discovery through Advanced Computing
OAK RIDGE National Laboratory