Unconventional pairing originating from disconnected Fermi surfaces in the iron-based oxypnictides

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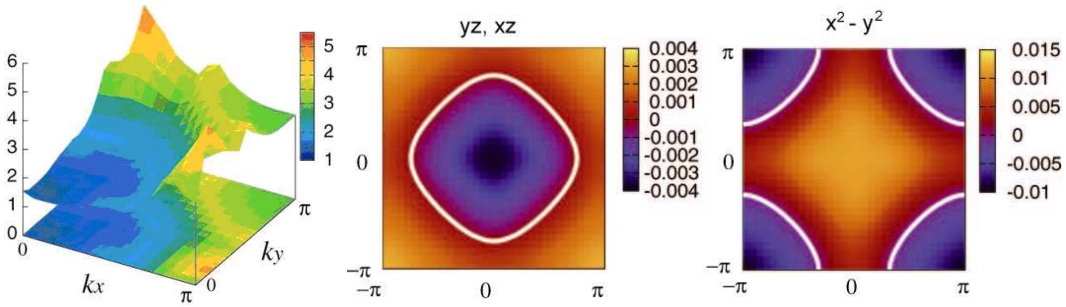
The iron-based $LaFeAsO_{1-x}F_x$ recently discovered by Hosono's group[1] is a fresh theoretical challenge as a new class of high-temperature superconductors. In order to clarify their mechanism of superconductivity, we have first constructed a tight-binding model in terms of the maximally localized Wannier orbitals from a first-principles electronic structure calculation, which has turned out to involve all the five Fe $3d$ bands[2]. This is used to calculate the spin and charge susceptibilities with the random phase approximation. The spin susceptibility has peaks around $k = (\pi, 0), (0, \pi)$ arising from a nesting across disconnected Fermi surface pockets (Fig., left panel), which is consistent with recent neutron scattering experiments. We have then plugged the susceptibilities into the linearized Eliashberg equation. For the doping concentration $x = 0.1$, we obtain an unconventional s-wave pairing with sign reversing gap functions. The gap function is actually a 5×5 matrix, for which the diagonal elements for dyz, dxz and $dx^2 - y^2$ orbitals are respectively shown (Fig., right panels). Experimental implications of the strong dependence of the gap between different orbitals will be discussed.



The present work is a collaboration with Kazuhiko Kuroki, Seiichiro Onari, Ryotaro Arita, Hidetomo Usui, Yukio Tanaka, and Hiroshi Kontani.

[1] Y. Kamihara, T. Watanabe, M. Hirano and H. Hosono, JACS **130**, 3296 (2008).
[2] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani and H. Aoki, cond-mat/0803.3325 (2008).