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Superconductivity in a unique type of copper oxide

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Table S1. Summary of the primary structure based on Rietveld refinements of Ba_2CuO_{4-y} from powder X-ray diffraction patterns at room temperature. The abbreviations of R_{wp} & R_p & χ^2 correspond to weight profile reliability factor, profile reliability factor, and match factor, respectively. U_{iso} is the isotropic atomic displacement parameter.

Formula: Ba_2CuO_{4-y} (T=300K); Space group: *I4/mmm* (No.139)

a = 4.0030(3) (Å); c= 12.942 (1) (Å);

R_{wp}: 3.41%; R_p: 2.47%; χ^2: 1.114

Atamic parameters

Atom	Wyckoff position	x	y	z	occupancy	U_{iso} ($*10^{-2}$ Å^2)
Ba	4e	0	0	0.35627(7)	1	1.66(6)
Cu	2a	0	0	0	1	1.51(9)
O1	4e	0	0	0.1438(6)	1	1.6(1)
O2	4c	0	0.5	0	0.592(15)	7(1)

Band structure of Ba_2CuO_4

To get some insight, the electronic energy band structure calculation in the local-density-approximation (LDA) is performed for an ideal Ba_2CuO_4 (nominal valence is Cu^{4+} ($3d^7$)) with the same lattice parameters as those of the present cuprate, a = 4.003 Å and c = 12.94 Å (d_A = 1.86 Å). The calculated band structure is displayed in **Fig. S1a** and is supportive of the multi-band nature of Ba_2CuO_4. There are two bands prevailing near the Fermi level (E_F), one with $3dz^2$ orbital character (blue) and the other with $3dx^2$-y^2 orbital character (red). Both bands almost completely overlap in energy, since the width of the dx^2- y^2 derived band is narrow due to the long in-plane Cu-O bond length. Even if E_F shifts up, in a rigid band manner, to the energy corresponding to a realistic hole density, somewhere between Cu^{3+} ($3d^8$) and Cu^{2+} ($3d^9$), both bands contribute nearly equally to the states near the Fermi level. The Fermi surface at the Fermi energy E_F corresponding to the Cu^{3+} ($3d^8$) filling is shown in **Fig. S1b**. Two types of Fermi surfaces are identified, one electron surface surrounding the Brillouin zone center (Γ) with $3dz^2$ orbital character (in blue) and one hole surface around the corner (M) of the zone with $3dx^2$-y^2 orbital character (in red). Basically the same calculation results have been reported in the Preprint at https://arXiv.org/abs/1809.04156 (2018), by Maier, T.A., Berlijn, T. & Scalapino, D.J. *d*-wave and $s^{\pm}$ Pairing Strengths in $Ba_2CuO_{3+\delta}$.

Fig. S1a

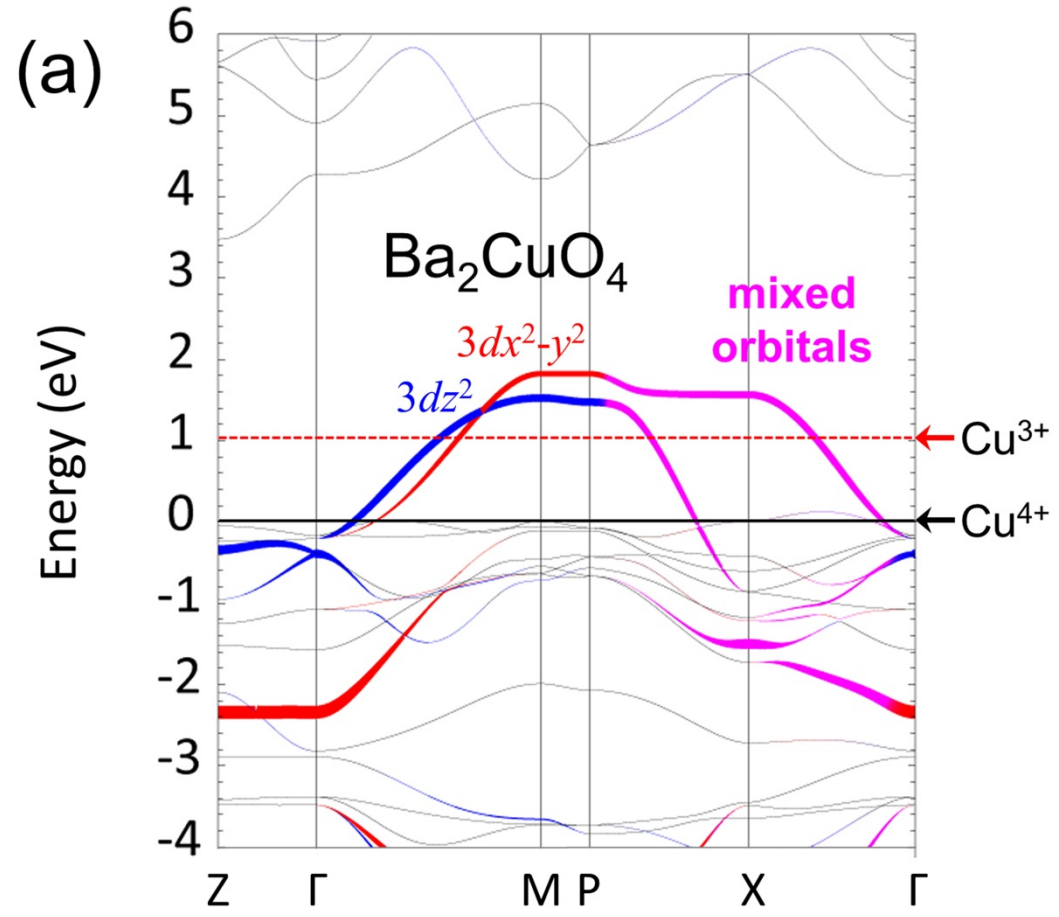
(a)
Ba2CuO4
mixed
orbitals
3dx2-y2
3dz2
Cu3+
Cu4+
Energy (eV)
6
5
4
3
2
1
0
-1
-2
-3
-4
Z
Γ
M
P
X
Γ

Fig. S1b