



Relationship between critical temperature and core orbital coupling in cuprate superconductors



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ABSTRACT

Because superconductivity and several relevant phenomena of high-temperature superconductors (HTSCs) arise from interactions of valence electrons near the Fermi surface, the valence orbital coupling has usually been thought to be critical to understanding the electronic pairing mechanism which seems work without the core coupling orbitals. But, as strong electronic correlations are believed to be essential for a comprehensive understanding of the cuprate superconductors, the Fermi surface is influenced directly or indirectly by all orbital couplings in the entire energy band. In this paper, we focused on the core orbital coupling which arises from the overlap between the Oxygen's 2s core orbital and the core p orbital of neighboring ion of CuO₂ layers as they have a similar energy level ranging from $-12 \sim -23$ eV below the Fermi level. The characters of this core coupling are varied with different kinds of neighboring ions or from the crystal structures. Based on the experimental superconducting critical temperature (T_c) data, we found that the binding energy differences between the valence couplings and the core couplings are positively related with the systemic T_c values for all cuprate superconductors. Obviously, this relationship suggests that the electron pairing nature of superconductivity for all cuprates might arise from the *sp* core orbital coupling.

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1. Introduction

Since the discovery of cuprate superconductors in 1986, one of the still open and challenging problems in condensed matter physics is the origin of the superconductivity in high-temperature superconductors (HTSCs). Decades of efforts based on thousands of experimental and theoretical researches pointed out that electron–electron interaction rather than the electron–phonon interaction plays the key role to trigger the superconductivity in HTSCs materials [1]. But, the unclear relationship between cuprate superconductivity and the electronic behavior remains an impediment to understanding the high transition temperature (T_c) superconducting mechanism [2]. Once the T_c rule with the isotope-effect coefficient was crucial in suggesting phonon-mediated pairing in the conventional low temperature superconductors and provided strong support for the BCS theory of superconductivity [3]. However, this is unlucky for the T_c rule with doping concentration in cuprate HTSCs: a T_c reaches a maximum value for an optimal doping [4]. In fact, considering that the doping concentration is almost the same value for different cuprate systems, as shown in

Fig. 1, this T_c rule shows limited information on its pairing mechanism. Obviously, the relationship between the maximum T_c and structural factors are essential for a complete understanding of the cuprate superconductors. Unless it is solved, there have been still such hot controversies on the understanding of the microscopic mechanisms of superconductivity in HTSCs [5,6].

2. Analysis and methods

As superconductivity arises from interactions of electrons near the Fermi surface (FS) in cuprates, the FS topology has usually been thought to be critical to understanding its pairing mechanism [2]. In addition, considering the practical complication of the model Hamiltonian treatment of many-body interactions [7], we could only work with a few valence orbital couplings, which lead us to ignore the interaction effect of other core orbital couplings below the Fermi level. In fact, as an electronically strong correlation system, the electronic interaction at the Fermi level would be affected directly or indirectly by all orbital couplings involving the whole electronic structure. Unless there are new research means, it seems that we have to adopt indirect theoretical or experimental routes [8]. Therefore, seeking for a real relationship between T_c and the energy band characters will play a key role on exploring the pairing mechanism.

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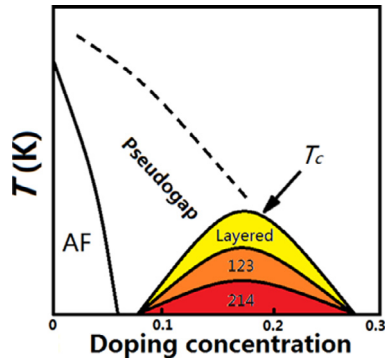


Fig. 1. A commonly known T_c rule for all vacancy doping cuprate superconductors. When the anti-ferromagnetic (AF) background of matrix is destroyed by vacancy doping concentration, T_c increases to reach a maximum at optimal doping before vanishing again at higher doping concentration. However, the peak values of T_c are quite different at a similar optimal doping concentration for different cuprate systems.

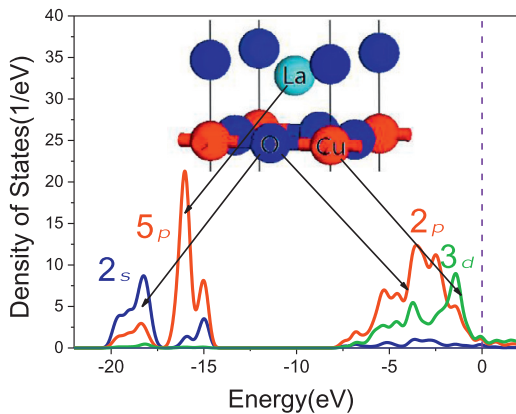


Fig. 2. The DOS diagram of La_2CuO_4 . Except for the valence coupling between the Cu 3d orbital and the O 2p orbital near Fermi level (0~–7 eV), there is also another core orbital coupling arising from the overlap between the O 2s core orbital and the p core orbital of the neighboring atom, in high binding energy (–12~–23 eV).

As shown in Fig. 2 (inserted), the CuO_2 planes are the key structure for all typical cuprates, in which copper and oxygen atoms form planes with the other atoms between them. Within each plane, the coppers arrange themselves in squares and the oxygens sit in between neighboring copper atoms. In addition, some important neighboring atoms such as Ca, Y, Sr, RE (La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) are adjacent to CuO_2 planes. Based on the density-of-states (DOS) curve calculated by means of Density Functional Theory (DFT) [9] in the Generalized Gradient Approximation (GGA), with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional [10] of the first-principles method, the energy band structure of cuprates were usually found to be mainly composed of O 2s and Cu 3d valence orbital coupling just below the Fermi level (around 0~–7 eV), as shown in Fig. 2. But except for the *pd* valence orbital couplings, there are also special core orbital *sp* couplings in all cuprate superconductors (around –12~–23 eV), which arise from the orbital overlap between the fulfilled O 2s and fulfilled p orbitals of the neighboring ion A of CuO_2 planes because they have a very close energy level [11]. What we discussed are the binding energy locations of main intensity peaks of two orbital couplings, which are influenced by the Fermi level even energy gap obtained from different DFT methods with or without local exchange-correlation potentials, but the variation of the energy difference of two couplings influenced by different methods is limited.

Table 1

Critical temperature T_c and the binding energy difference ΔE [15] for most cuprate superconductors.

	Compounds	Structure	ΔE (eV)	T_c (K)
1	TlBaSrCuO ₅	TI-1201	13.5	56.5 [16]
2	TlBa ₂ CaCu ₂ O ₇	TI-1212	15.1	82 [17]
3	TlBa ₂ Ca ₂ Cu ₃ O ₉	TI-1223	18.6	133 [18]
4	TlBa ₂ Ca ₃ Cu ₄ O ₁₁	TI-1234	18.6	127 [19]
5	Tl ₂ Ba ₂ CuO ₆	TI-2201	15.7	90 [17]
6	Tl ₂ Ba ₂ CaCu ₂ O ₈	TI-2212	16.5	110 [17]
7	Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀	TI-2223	18.8	128 [20]
8	Tl ₂ Ba ₂ Ca ₃ Cu ₄ O ₁₂	TI-2234	18.4	119 [21]
9	Bi ₂ Sr ₂ CuO ₆	Bi-2201	12.7	34 [22]
10	Bi ₂ Sr ₂ CaCu ₂ O ₈	Bi-2212	16.2	96 [23]
11	Bi ₂ Sr ₂ Ca ₂ Cu ₃ O ₁₀	Bi-2223	16.0	110 [17]
12	Bi ₂ Sr ₂ Ca ₃ Cu ₄ O ₁₂	Bi-2234	16.6	110 [24]
13	HgBa ₂ CuO ₄	Hg-1201	16.0	97 [17]
14	HgBa ₂ CaCu ₂ O ₆	Hg-1212	18.5	128 [17]
15	HgBa ₂ Ca ₂ Cu ₃ O ₈	Hg-1223	18.8	135 [25]
16	HgBa ₂ Ca ₃ Cu ₄ O ₁₀	Hg-1234	18.7	125 [26]
17	Sr _{0.9} La _{0.1} CuO ₂	IL	13.4	43 [27]
18	Sr _{0.7} Ca _{0.3} CuO ₂	IL	16.1	99 [28]
19	YBa ₂ Cu ₃ O ₇	123-O	16.3	92 [29]
20	LaBa ₂ Cu ₃ O ₇	123-O	16.5	93 [30]
21	PrBa ₂ Cu ₃ O ₇	123-O	15.5	92 [31]
22	NdBa ₂ Cu ₃ O ₇	123-O	15.6	96 [29]
23	SmBa ₂ Cu ₃ O ₇	123-O	15.7	93.5 [32]
24	EuBa ₂ Cu ₃ O ₇	123-O	15.7	95.0 [33]
25	GdBa ₂ Cu ₃ O ₇	123-O	16.0	94.5 [34]
26	DyBa ₂ Cu ₃ O ₇	123-O	16.3	95.1 [35]
27	HoBa ₂ Cu ₃ O ₇	123-O	16.4	92.9 [32]
28	ErBa ₂ Cu ₃ O ₇	123-O	16.4	92.4 [32]
29	TmBa ₂ Cu ₃ O ₇	123-O	16.3	92.5 [32]
30	YbBa ₂ Cu ₃ O ₇	123-O	16.3	96.1 [35]
31	LuBa ₂ Cu ₃ O ₇	123-O	16.5	92.4 [35]
32	La ₂ CuO ₄	214-T	12.5	41.5 [36]
33	La _{1.85} Sr _{0.15} CuO ₄	214-T	13.0	36 [37]
34	La _{1.85} Ba _{0.15} CuO ₄	214-T	13.2	43 [38]
35	Nd _{1.85} Ce _{0.15} CuO ₄	214-T*	13.3	24 [39]
36	Nd _{1.32} Ce _{0.41} Sr _{0.27} CuO ₄	214-T*	13.4	24 [40]

As the orbital couplings have different widths depending upon the degree of overlap in the atomic orbitals from which they arise, the band widths associated with core orbitals are usually narrow due to the small overlap between adjacent atoms, but the cuprate seems to be a large core coupling as a result of a large band width, even as wide as that of the valence coupling according to the calculated DOS Curves. Actually the core orbital coupling is very common in cuprates. The characters of this coupling are mainly varied with either the different structures of superconductors or the different kinds of A ion. However, these characteristic core couplings are seldom mentioned, as for the reason that is discussed in the above paragraph.

From crystal structure characters and their experimental T_c data in Table 1, the main typical cuprates usually are classified as three classes: La-214 with a smaller T_c , RE-123 with a mediate T_c and the Ca-multiple layers with a larger T_c . Their CuO_2 planes are similar in terms of atomic structure, but the main difference comes from both the kind and amount of neighboring ions.

In Fig. 3(a), based on the DFT's DOS calculation, it is shown that the most characteristic difference in DOS comes from the energy position and height of the core orbital coupling. Among these core couplings, most intensity peaks in the core orbital couplings are respectively La 5p, O 2s and Ca 3p responding to La-214, RE-123 and Ca-Multiple layers, which are located at around –15, –17 and –19 eV respectively as shown in Fig. 3(a). Therefore, the important characters in their DOS curves also come mainly from these core orbital couplings.

In Fig. 3(b), as the RE's core p orbital is smaller in intensity than Oxygen's core 2s orbital (the “weight center” of core orbital

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