Band structure trends of hole-doped cuprates and correlation with T_c max

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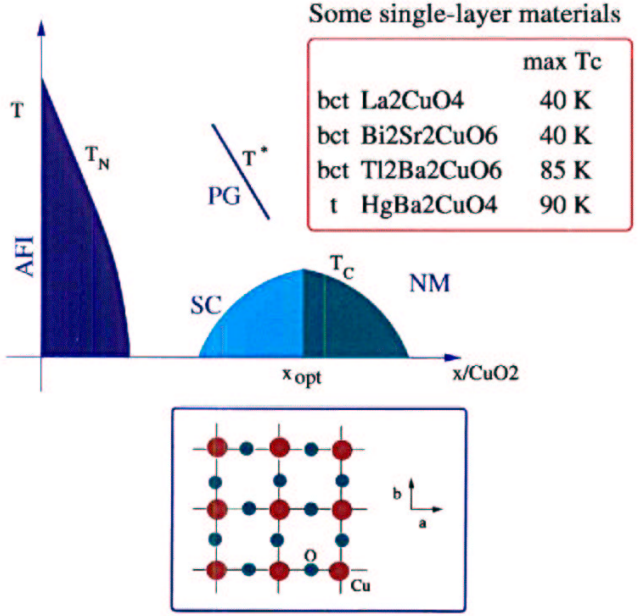
Motivation

why is T_c at optimal doping material dependent?



Some single-layer materials

		max Tc
bct	La2CuO4	40 K
bct	Bi2Sr2CuO6	40 K
bct	Tl2Ba2CuO6	85 K
t	HgBa2CuO4	90 K

material dependence → electronic structure

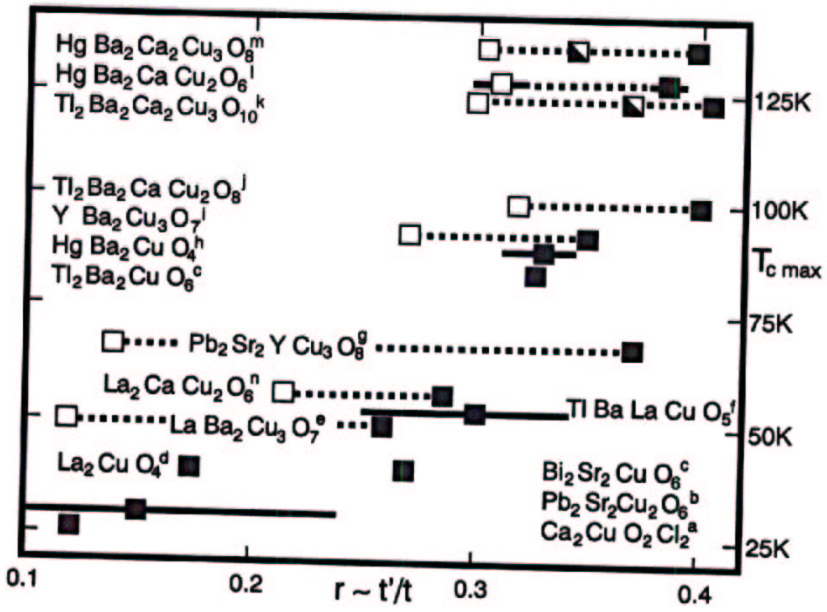
→ hopping integrals $H_0 = \sum t_{ij} c_i^\dagger c_j$

model Hamiltonian $H = H_0 +$ Coulomb $+ \ldots$

Parameters of one-band model

15 HTSC with 1-3 layers

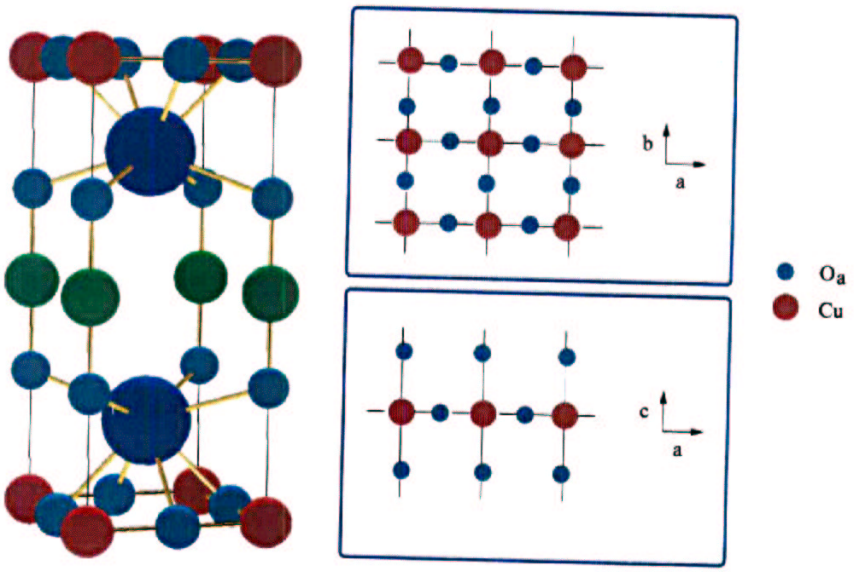
tetragonal and bct (LTO) structures



Correlation between calculated r and observed max T_c.

Filled squares: Single layer materials and most bonding subband for multilayers. *Empty squares*: Most antibonding subband. *Full lines*: k_z dispersion for tetragonal materials

HTSC: $HgBa_2CuO_4$

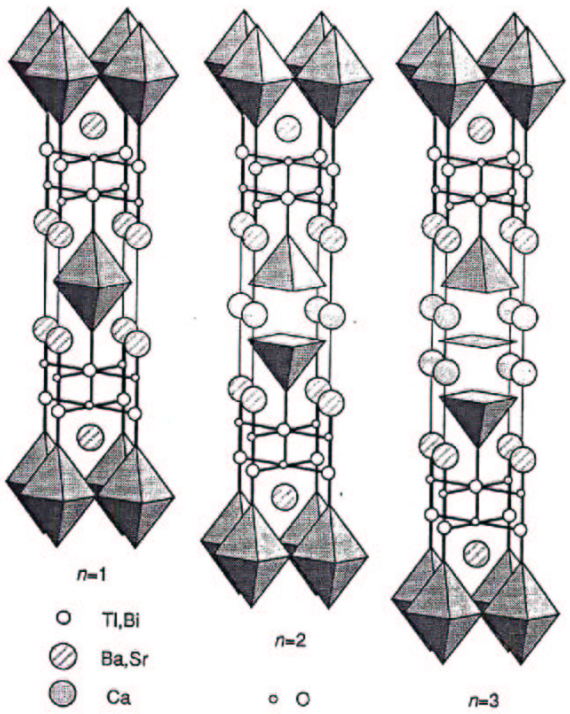


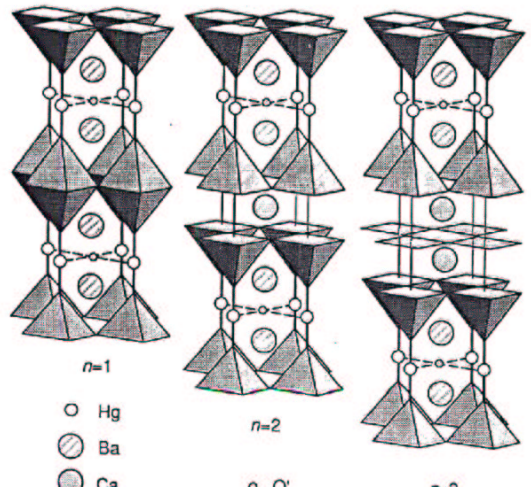
Cu - O_a : 1.93 Å

Cu - O_c : 2.79 Å

Hg - O_c : 1.95 Å

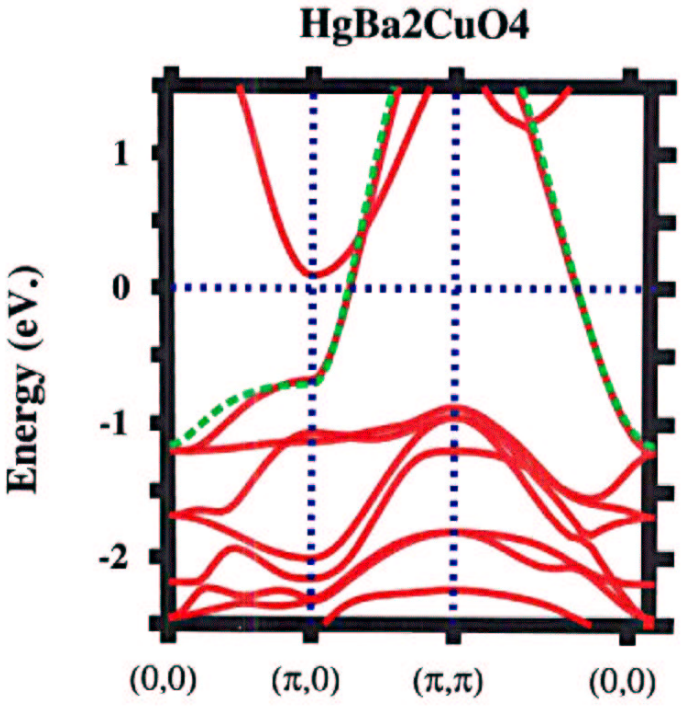
MPI-FKF Stuttgart



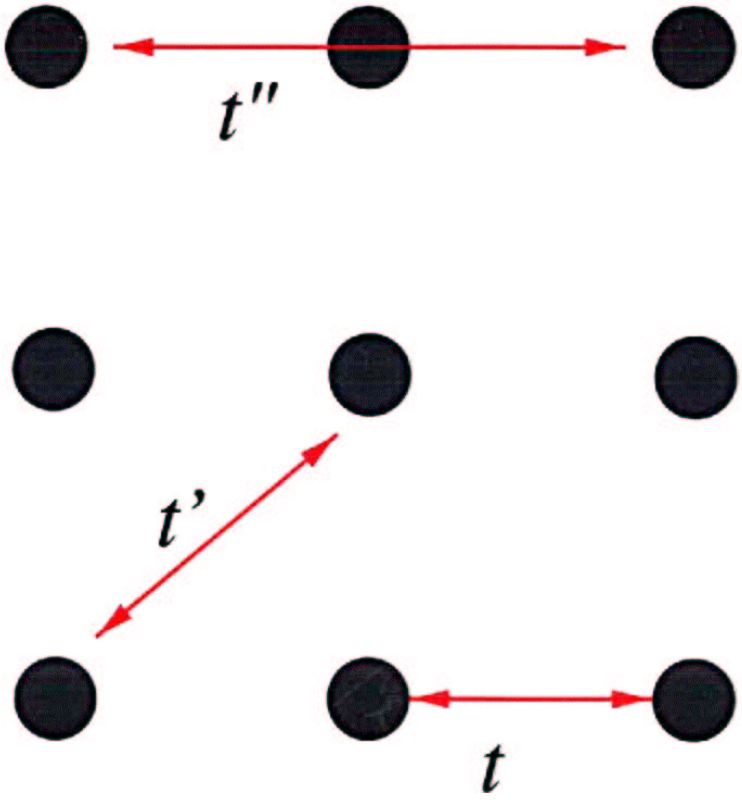


Single CuO2 layer materials

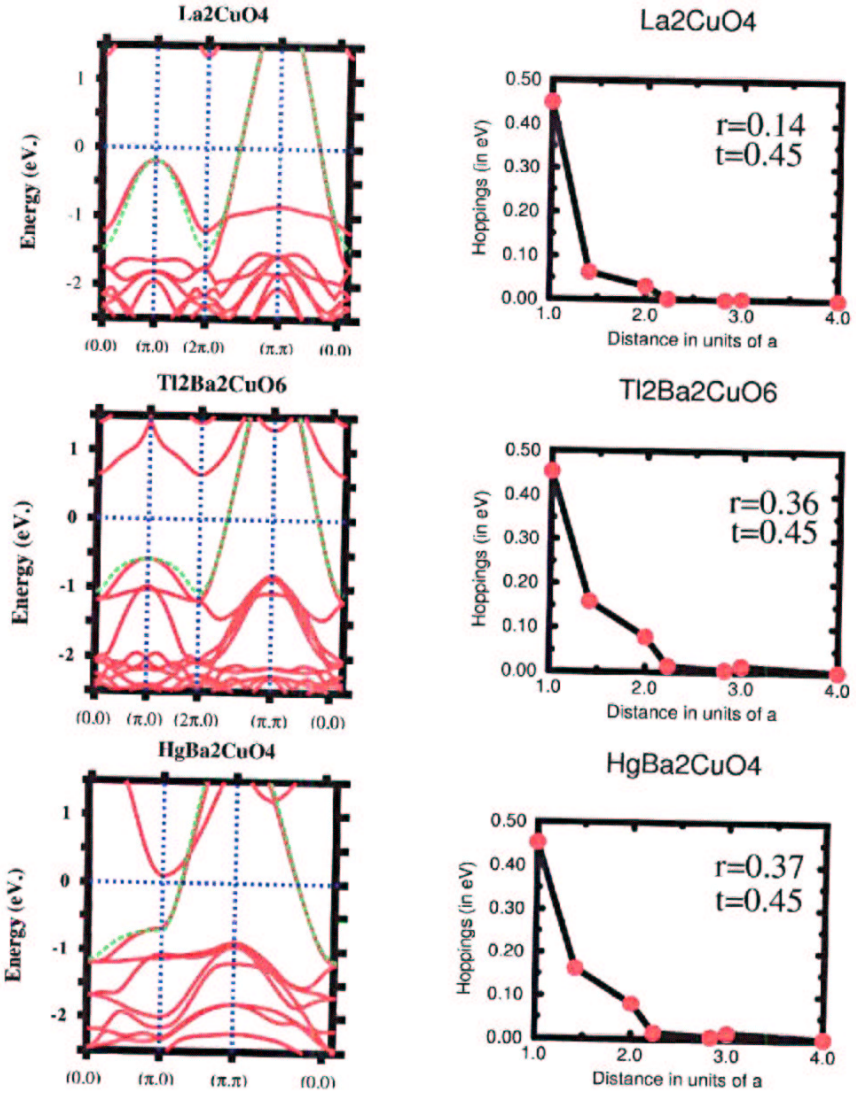
From LDA ⟶ one band TB model

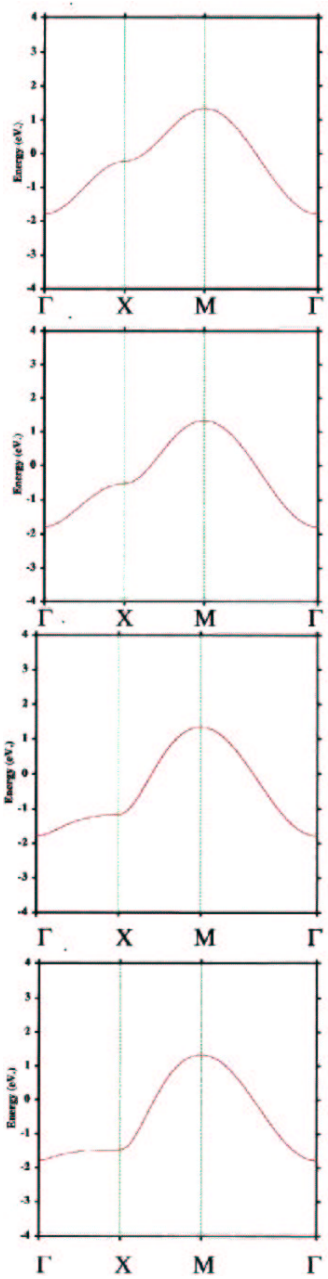


CuO2 plane: Hopping integrals

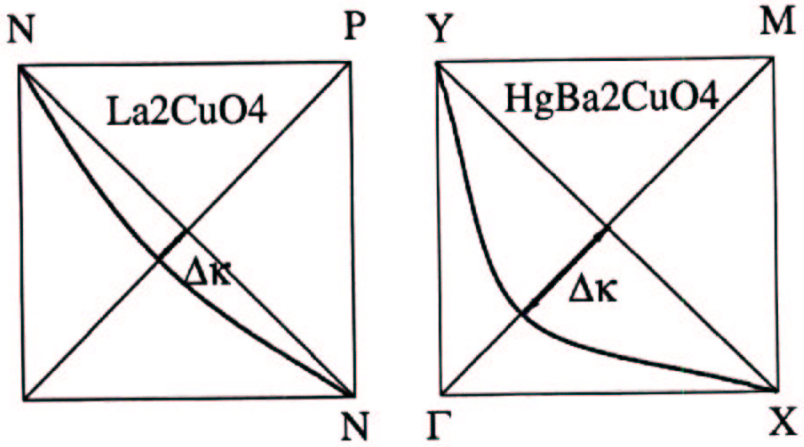


LDA bands, low energy conduction band and hopping integrals





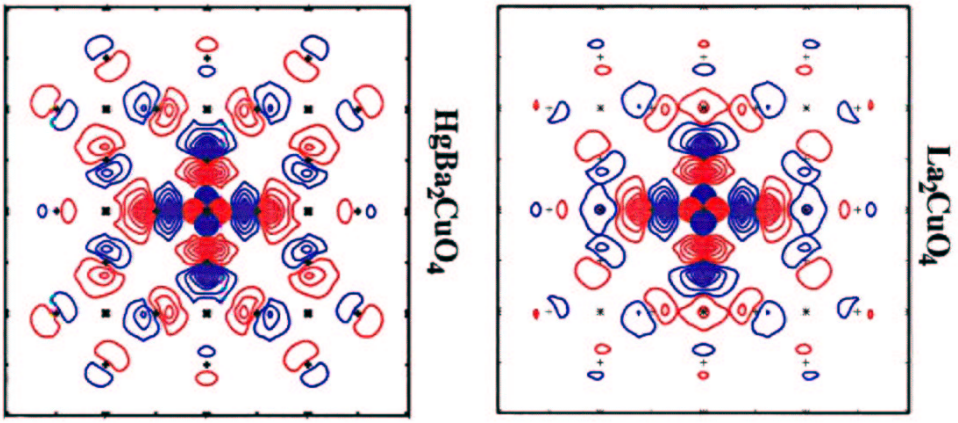
Constant energy contours passing through the $(\pi, 0)$ saddle point



Materials-dependence contained in a single parameter

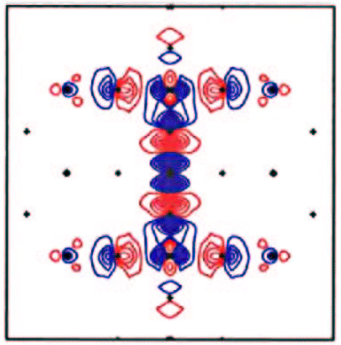
$$r = \frac{1}{2}\sin\left(\frac{\Delta k}{\Gamma - M}\right) \sim \frac{t'}{t}$$

Conduction-band orbital in the CuO_2-layer for La_2CuO_4 and $HgBa_2CuO_4$

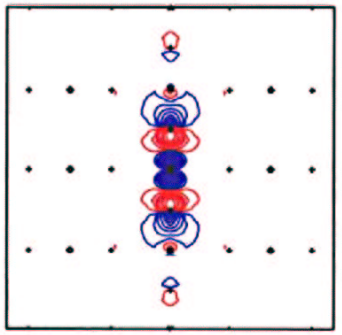


Conduction-band orbital in the xz-plane

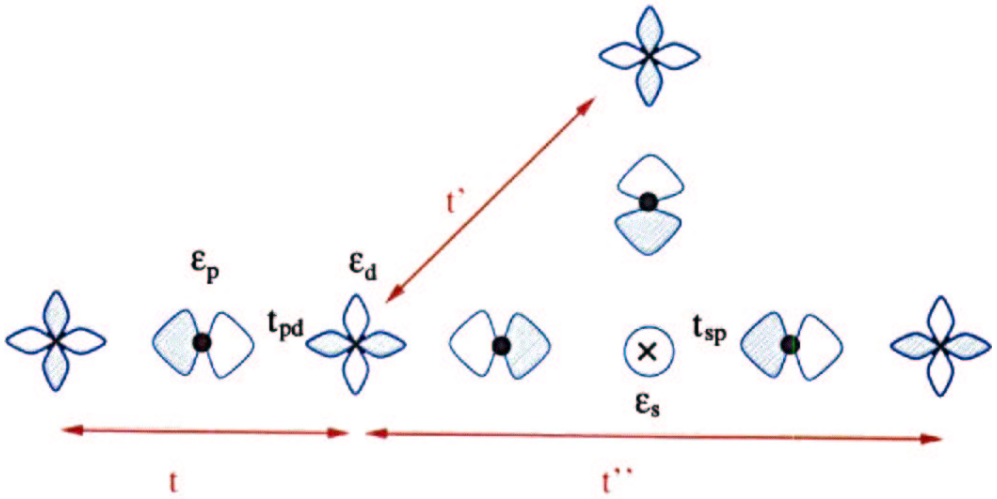
La_2CuO_4

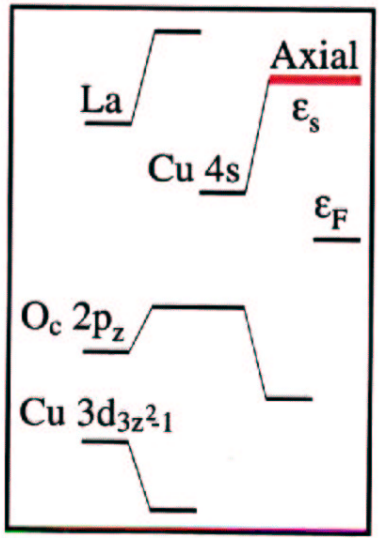


$HgBa_2CuO_4$



From one- to four-band model





One-band model

$$\epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) + 4t'\cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) + \dots$$

with $t'/t = r + o(r)$

Four-band model

$$\epsilon(\mathbf{k}) = \frac{2t_{pd}^2}{\epsilon_F - (\epsilon_p + \epsilon_d)/2}\left(u + \frac{2rv^2}{1-2ru}\right)$$

with $\begin{matrix} u \\ v \end{matrix}\} = (\cos k_x \pm \cos k_y)$

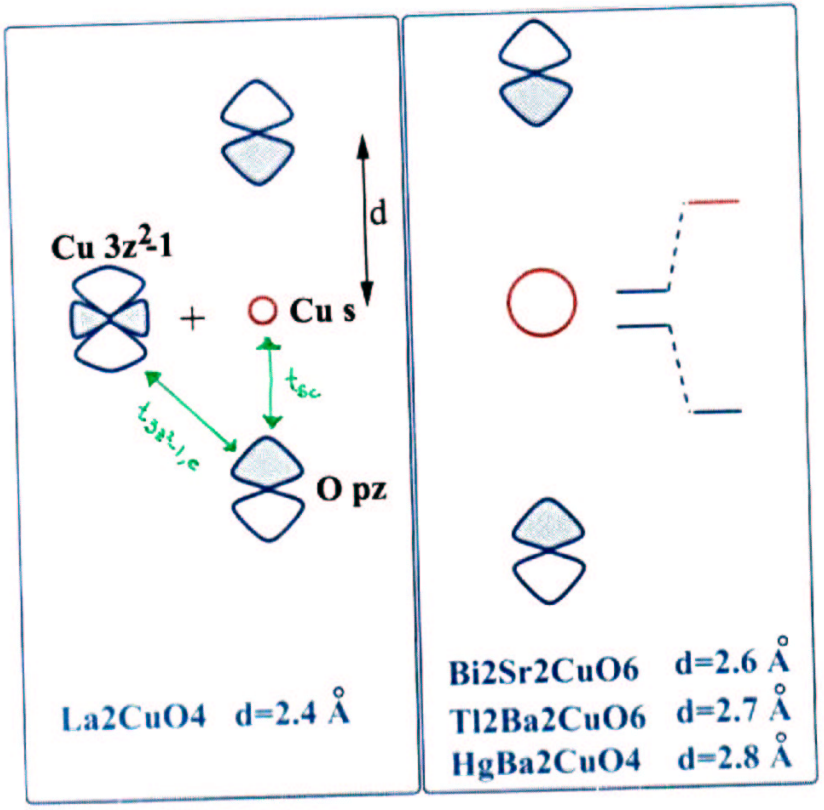
$r = [2(1+s)]^{-}1$, and $s = (\epsilon_s - \epsilon_F)(\epsilon_F - \epsilon_p)/(2t_{sp}^2)$

The range-parameter is essentially the Cu s character

$$|c_s|^2 \propto v^2 r^2 |c_d|^2$$

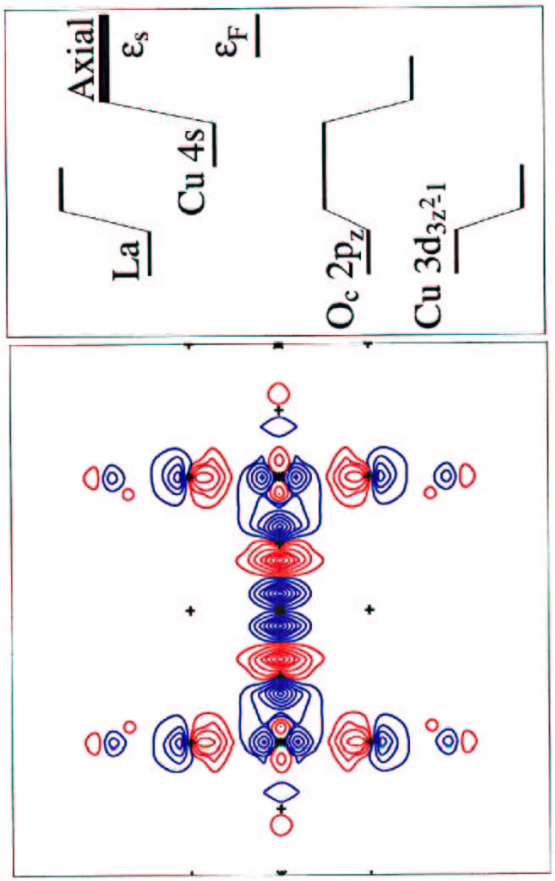
The axial orbital

Effective Cu s: Cu s +apical O_c p_z + Cu d_{3z^2-1}



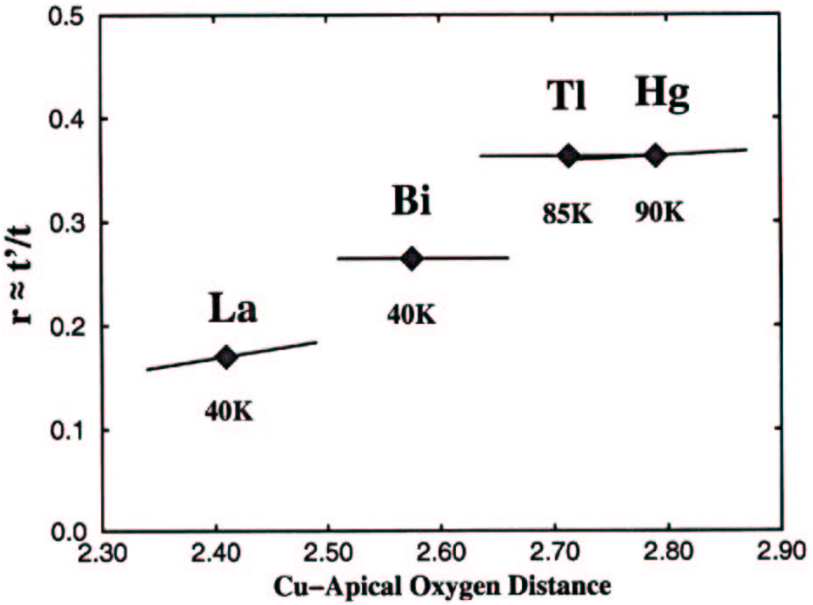
$t_{3z^2-1,c} \propto d^{-4}$ $t_{sc} \propto d^{-2}$

Axial orbital: La_2CuO_4



Parameters of one-band model

single-layer materials



r is controlled by the distance from Cu to apical O and the bonding of apical O to La, Bi, Tl or Hg.

Dimpling

- it does not influence the range of the intralayer hopping
- it reduces t through admixture of $O_{a/b}$ p_z
- it reduces t_{pd}
- it opens a new channel for interlayer coupling ($t^{\perp}_{zz}$) in multilayer systems.

Interlayer coupling

The hopping integral $t_\perp$ proceed via the axial orbital

- tetragonal materials (eg. $HgBa_2CuO_4$)

$$t_\perp \sim r^2 v^2 \cos ck_z \qquad v \equiv \frac{1}{2}(\cos k_x - \cos k_y)$$

The CuO_2 layers are stacked on top of each other $\longrightarrow$ the interlayer coupling proceed from apical O at $(0,0,zc)$ via Hg $6s/6p_z$ at $(0,0,c/2)$ to apical O at $(0,0,(1-z)c)$.

- bct materials (eg. La_2CuO_4)

$$t_\perp \sim r^2 v^2 \cos \frac{1}{2}k_x \cos \frac{1}{2}k_y \cos \frac{1}{2}ck_z$$

The interlayer coupling proceed by hopping from apical O at $(0,0,zc)$ to its four nearest neighbors apical O at $(\pm 1/2, \pm 1/2, (1/2-z)c)$.

$\longrightarrow$ Interlayer coupling makes ϵ_s dependent on k_z

Interpretation and Trends

- The only material dependent parameter is the energy ϵ_s of the axial orbital. This energy is $\epsilon_s - \epsilon_{x^2-y^2} \sim 6-9$ eV.

- The hopping integrals $t', t'' \ldots$, as well as $t_\perp$ proceed via this effective Cu 4s orbital

$$t'/t \sim r \qquad t''/t' \sim 1/2 \qquad r \equiv r(\epsilon_s)$$

$$t_\perp \sim r^2 v^2 \cos ck_z \qquad v \equiv \frac{1}{2}(\cos k_x - \cos k_y) \quad \text{tetragonal}$$

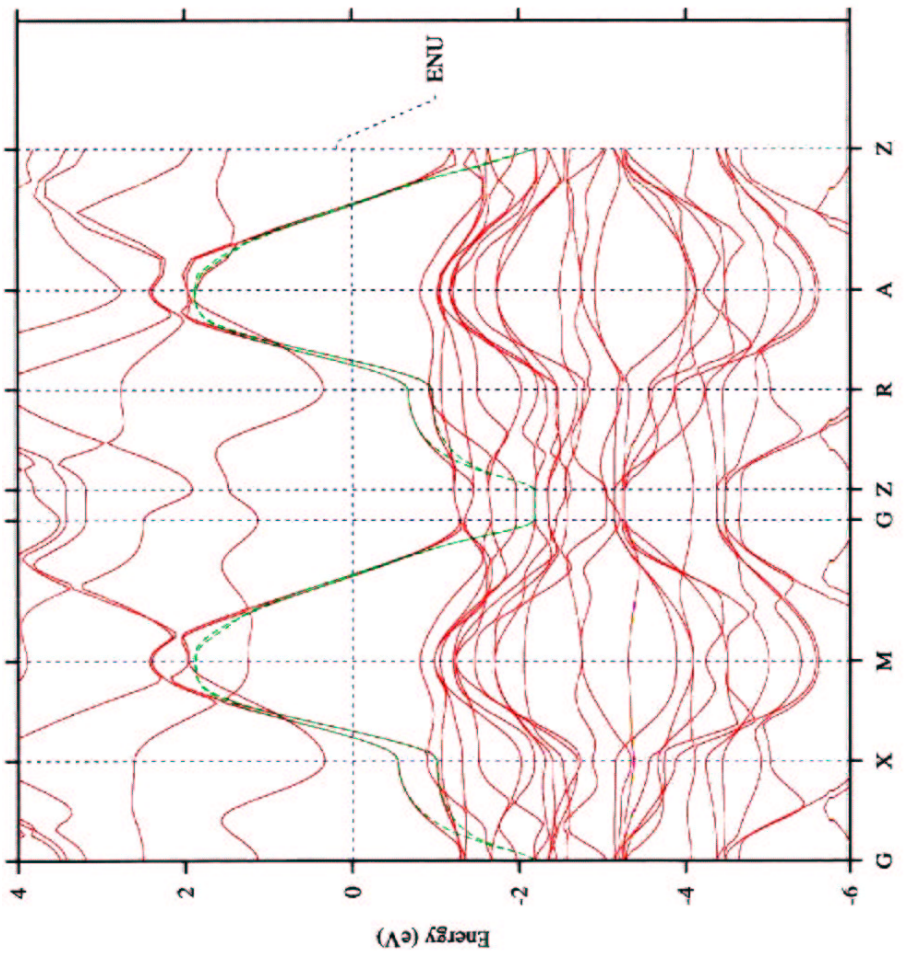
$$t_\perp \sim r^2 v^2 \cos \frac{1}{2}k_x \cos \frac{1}{2}k_y \cos \frac{1}{2}ck_z \quad \text{bct}$$

- One of the most important structural parameters determining the normal and superconducting properties for single layer materials is the distance between the apical oxygen and the plane copper.

Materials with multiple CuO2 layers

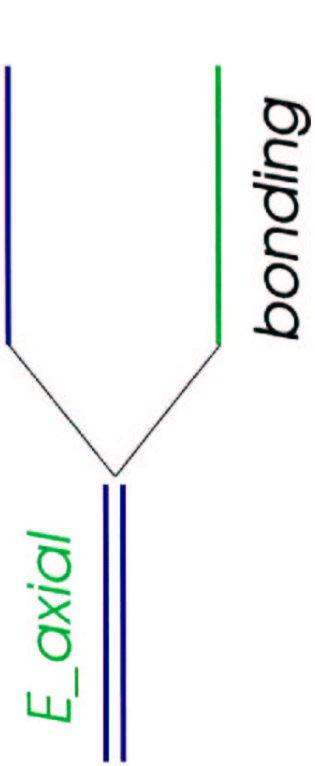
each CuO2 layer == one band

hoppings for different bands are different

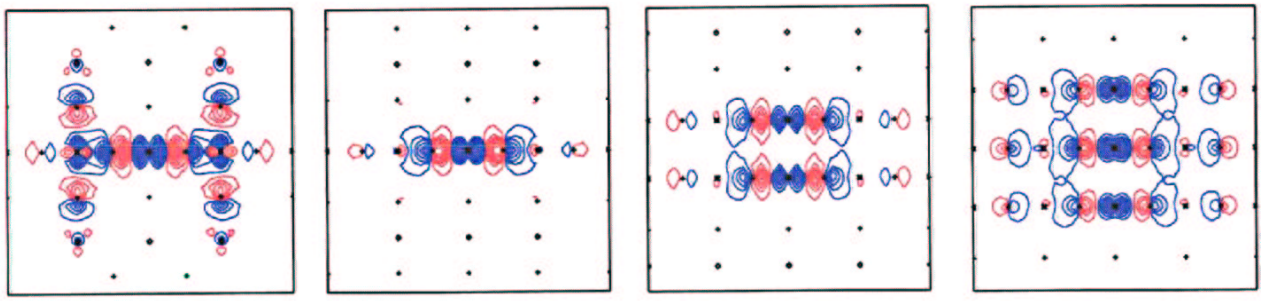


Axial Orbital

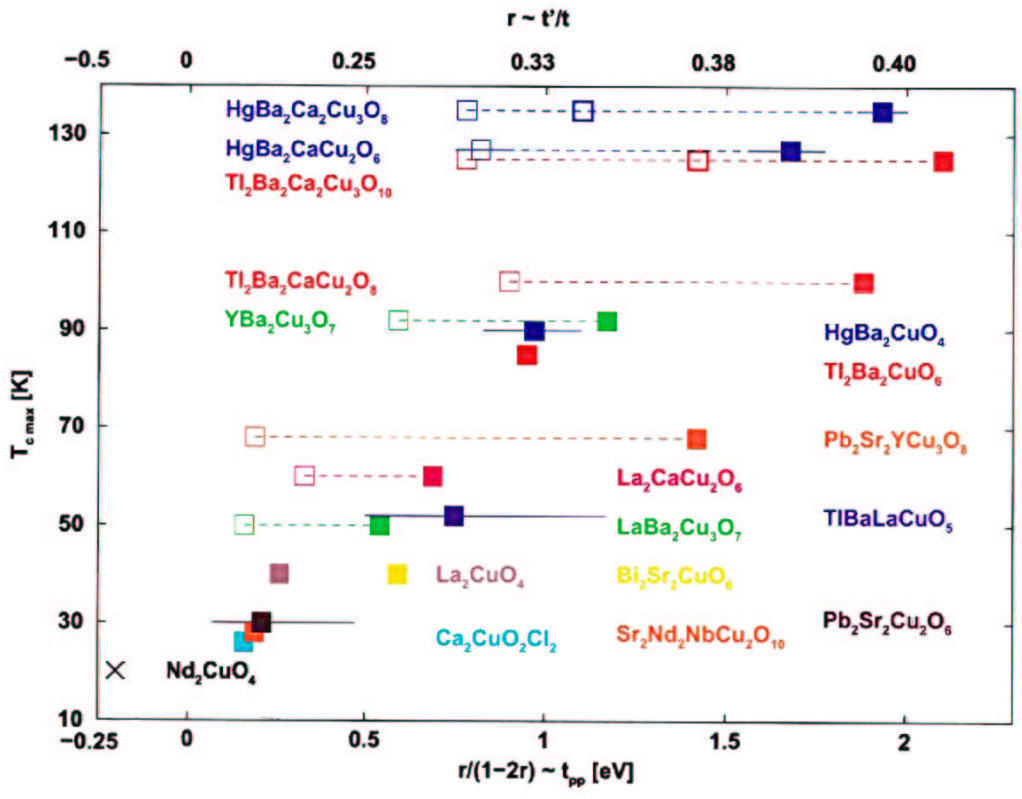
Two CuO2 layers



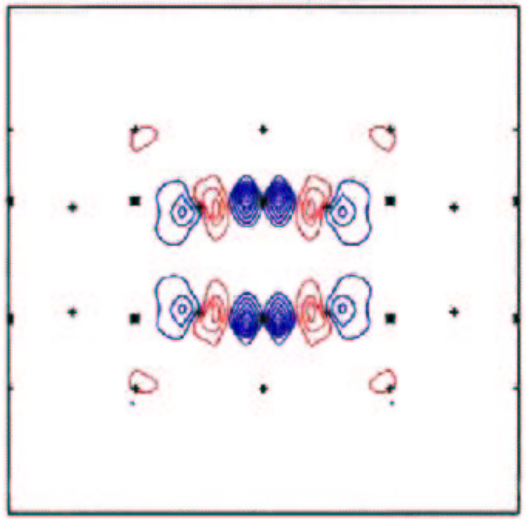
Conduction-band orbital in the xz-plane



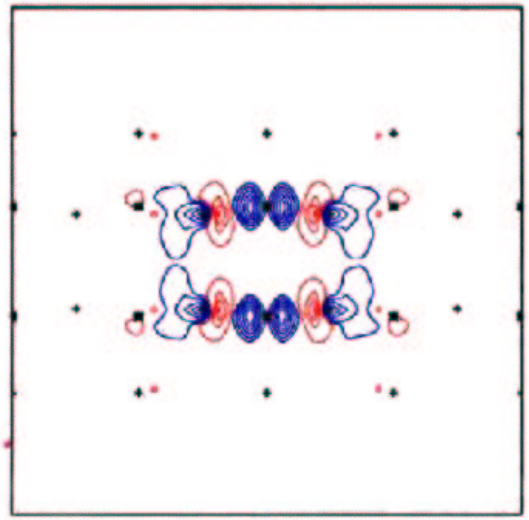
La_2CuO_4 $HgBa_2CuO_4$ $HgBa_2CaCu_2O_6$ $HgBa_2Ca_2Cu_3O_8$



$LaBa_2Cu_3O_7$



$YBa_2Cu_3O_7$



Interlayer coupling

In multilayer systems the interlayer hopping $t_\perp$ is due to

- flat layers
  - Cu s - Cu s hopping integrals $t_{ss}^\perp$

    $\longrightarrow t_\perp \propto t_{ss}^\perp(\cos(k_x) - \cos(k_y))^2$

- dimpled/buckled layers
  - Cu s - Cu s hopping integrals $t_{ss}^\perp$
  - plane O p_z - plane O p_z hopping integrals $t_{zz}^\perp$

Conclusions

- We have identified an electronic parameter – the range parameter – which correlates with the observed T_C max.
- this correlation holds for essentially all hole-doped HTCS materials and should be a useful guide for materials synthesis and a key for understanding the mechanism of HTCS
- range parameter $r \leftrightarrow$ energy axial orbital
- The range parameter controls the hopping integrals beyond nn in the plane $(t', t'', \ldots)$ and the hopping integral perpendicular to the plane $(t_\perp)$.
- no support to Van Hove scenario or the interlayer-pair-tunneling mechanism.

Speculations as to why increase of the in-layer hopping range causes $T_{c\,max}$ to increase

- A large range parameter increases the diagonal hopping $t' \longrightarrow$ suppresses static stripe order.
- A large range parameter leads to better screening the Coulomb repulsion.
- In-layer coherence is strengthened, coupling to apical oxygen and insulating layer is weakened.
- The propensity to buckling is increased.

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