Hole-doped HTSCs: band structure trend, contact field and correlation with T_c max

E. Pavarini[1,2], I. Dasgupta[3,2], T. Saha-Dasgupta[4,2], O. Jepsen[2], O.K. Andersen[2]

1- Dipartimento di Fisica "A. Volta", Via Bassi 6, I-27100 Pavia

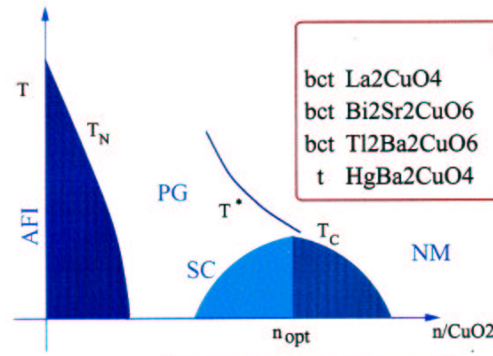
2- MPI-FKF, Heisenbergstrasse 1, 70569 Stuttgart, Germany

3- IIT Bombay, Mumbay 400 076, India

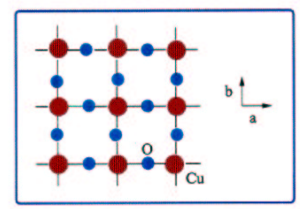
4- SN Bose National Centre for Basic Sciences, Kolkata 700098, India

A. Volta Pavia

Motivation



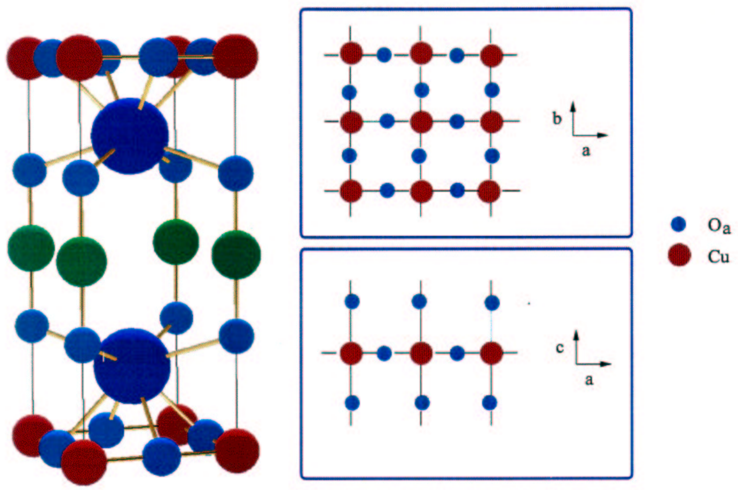
	max Tc
bct La2CuO4	40 K
bct Bi2Sr2CuO6	40 K
bct Tl2Ba2CuO6	90 K
t HgBa2CuO4	90 K



Electronic structure $\rightarrow H = \sum t_{ij} c_i^\dagger c_j$

MPI-FKF Stuttgart

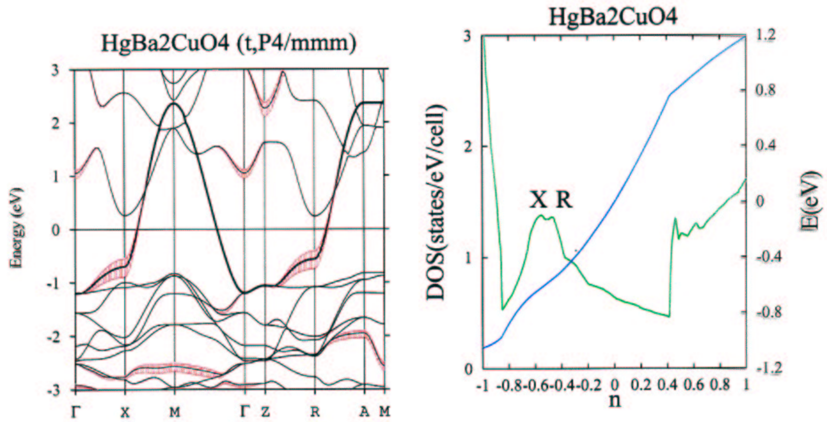
HTSC: $HgBa_2CuO_4$



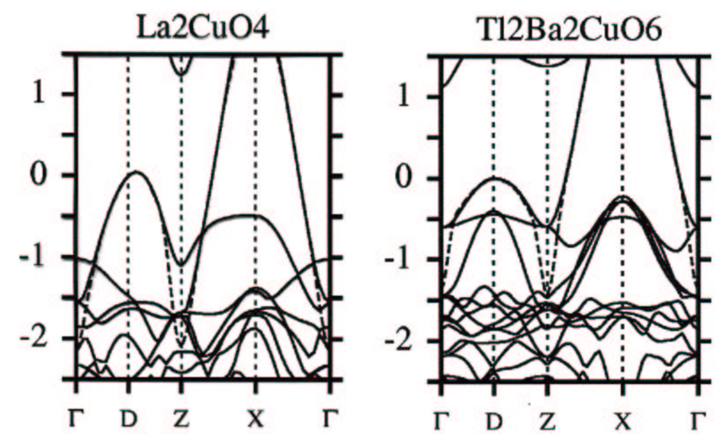
Cu - O_a : 1.93 Å
Cu - O_c : 2.79 Å
Hg - O_c : 1.95 Å

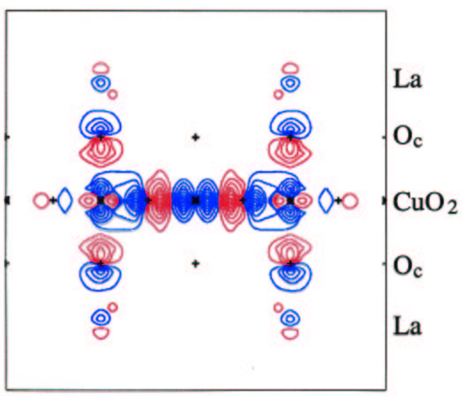
Electronic structure

DFT(LDA), TB LMTO method.



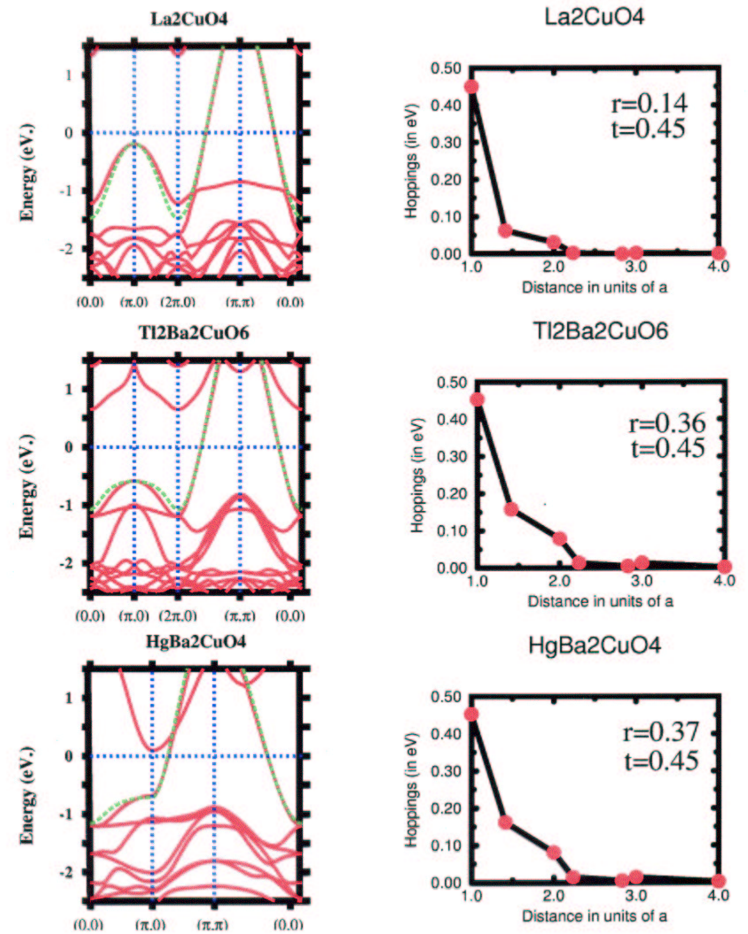
LDA bands → one-band model



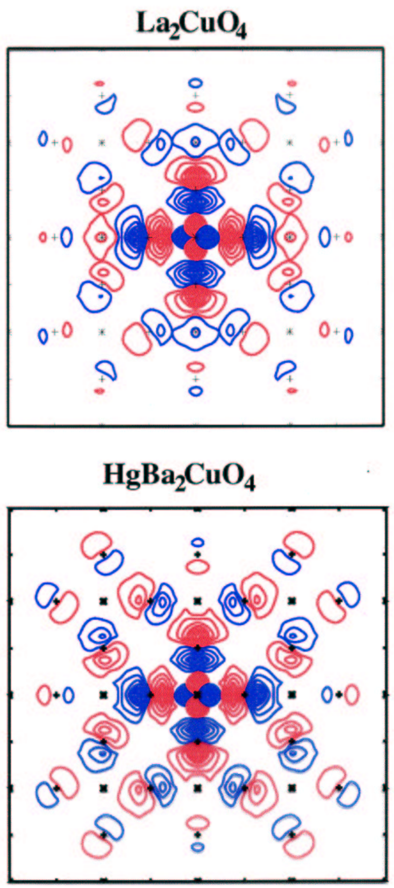


method: O.K. Andersen et al, Phys Rev B 62, R16219 (2000)

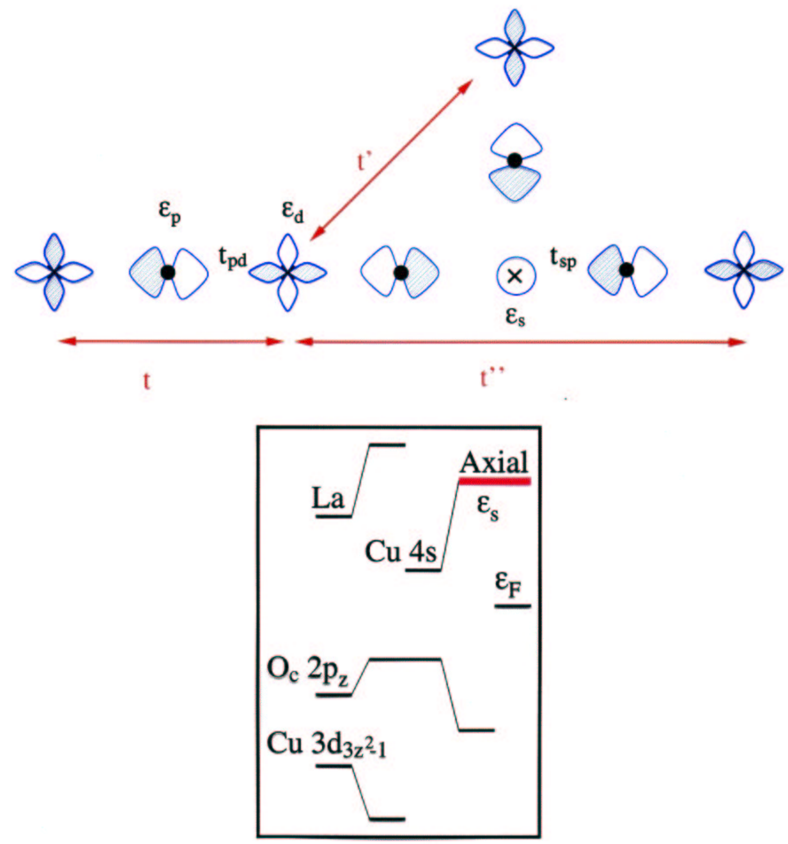
LDA bands, low energy conduction band and hopping integrals



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



From one- to four-band model



One-band model

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

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 $\left.{u \atop v}\right\} = (\cos k_x \pm \cos k_y)$

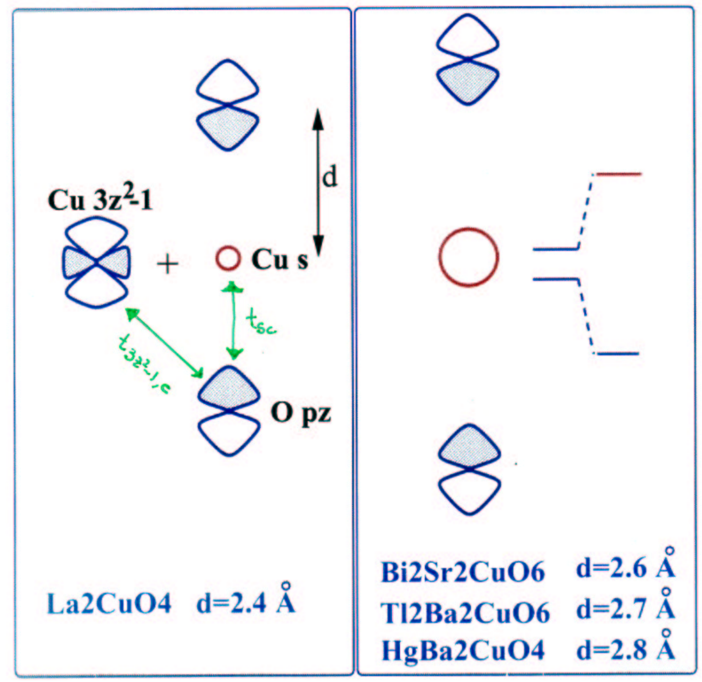
$r = [2(1+s)]^{-1}$, and $s = (\epsilon_s - \epsilon_F)(\epsilon_F - \epsilon_p)/(2t_{sp}^2)$

The range-parameter is essentially the Cu s character

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

The axial orbital

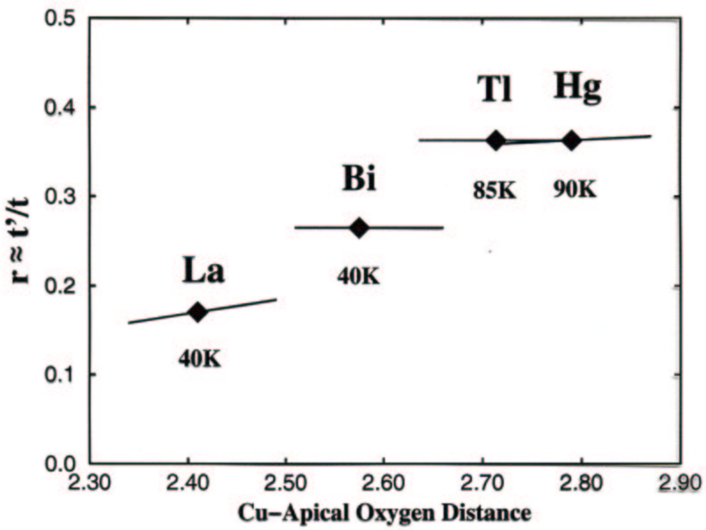
Effective Cu s: Cu s +apical O_c p_z + Cu d_{3z^2-1}



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

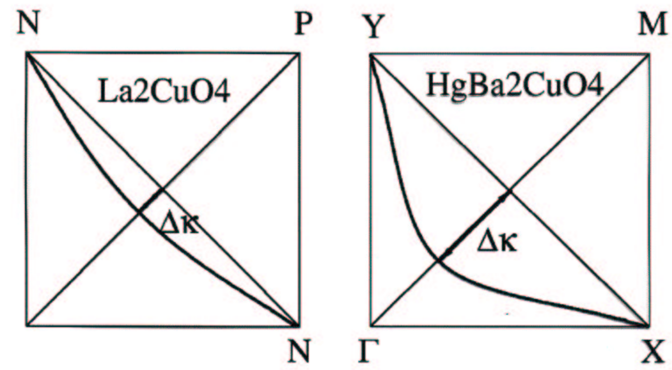
Parameters of one-band model

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.

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



Materials-dependence contained in a single parameter

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

Interpretation and Trends

- The only material dependent parameter is the energy ϵ_s of the effective Cu 4s orbital (axial orbital). This energy is $\epsilon_s - \epsilon_{x^2-y^2} \sim 6-9$ eV.

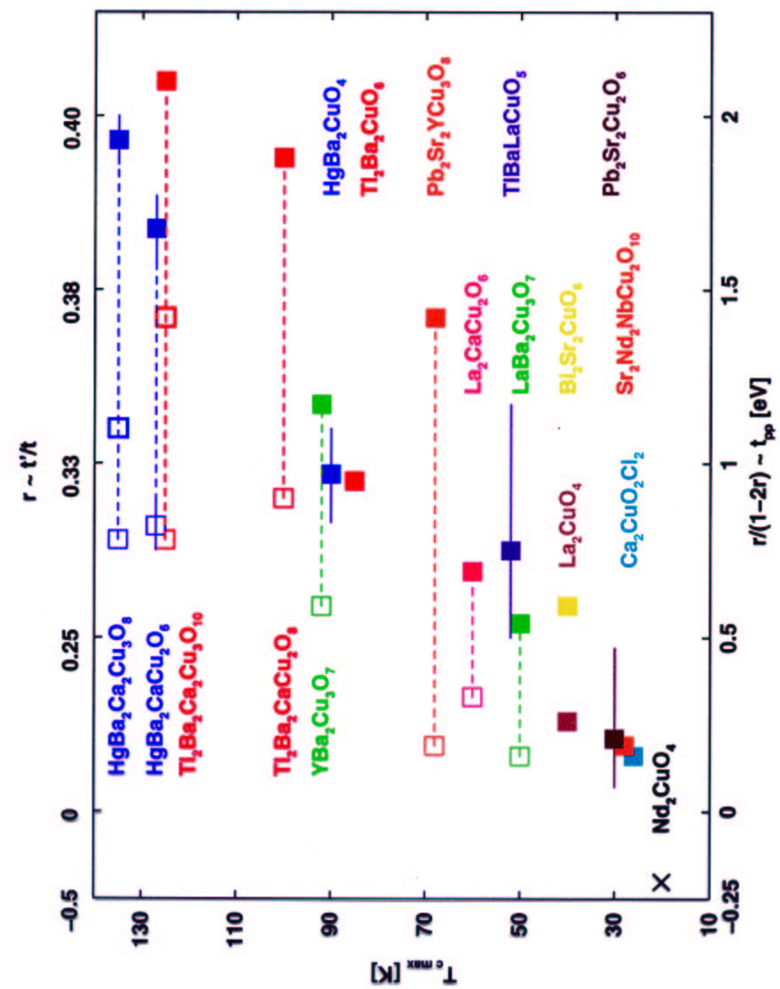
- The hopping integrals $t', t'' \ldots$, as well as $t_\perp$ proceed via this effective Cu 4s orbital

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

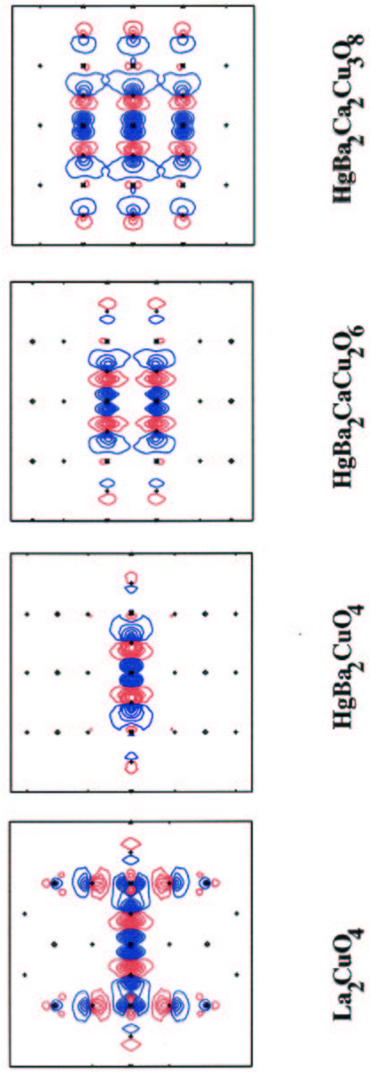
$$t_\perp \sim r^2 v^2 \cos ck_z \quad v \equiv \frac{1}{2}(\cos k_x - \cos k_y) \quad \text{tetragonal}$$

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

- 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.



Conduction-band orbital in the xz-plane



Interpretation and Trends

- The essential material-dependence is contained in a single parameter, r, which expresses the range of the intra-layer hopping, $t'/t \sim r + o(r)$.
- This parameter is controlled by the axial orbital, the effective Cu 4s, $\epsilon_s - \epsilon_{d_{x^2-y^2}} \sim 6 - 9eV$.
- The axial orbital is a hybrid between Cu $4s$, Cu $3d_{3z^2-1}$, apical oxygen $2p_z$ and farther orbitals such as Hg or La.
- The ratio of axial-orbital to Cu $d_{x^2-y^2}$ character is proportional to $r^2(\cos k_x - \cos k_y)^2 = r^2 v^2$
- The materials with larger r tend to be those with the higher observed value of max T_c. For the materials with the highest observed max T_c, the axial orbital is almost pure Cu $4s$.
- The correlation between r and max T_c holds also for multilayers with $n \leq 3$, if electrons are assumed to be coherent across the multilayer and if we use the r-value for the Cu $4s$ **bonding** subband.

- The axial orbital is also the main vehicle for perpendicular hopping. The axial character is maximum at "hot spots" and vanishes at cold "spots".

- CuO_2 layers stacked on top of each other: $t_\perp(\mathbf{k}) \propto v^2 \cos k_z$. bct stacked CuO_2 layers: additional nodes along $k_x = \pi \longrightarrow k_z$-dispersion killed in single-layer Tl but not in single-layer Hg, nearly same max T_c. This argues against pair-tunnelling as a mechanism for boosting T_c.

Experiments consistent with our results

- Fermi surface shape: ARPES of La_2CuO_4 (overdoped), YBa_2CuO_7 and $Bi_2Sr_2CaCu_2O_8$

- T_c in $La_{1.9}Sr_{0.1}CuO_4$ films with different degrees of strain, J.-P. Locquet et al., Nature **394**, 453 (1998)