# Oxygen Partial Density of States in YBa$_2$Cu$_3$O$_{7-\delta}$ (YBC)

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We investigate plain versus chain superconductivity in YBC by calculating the partial density of electronic states associated with plane O2, O3 and chain O1, O4 oxygen atoms. The results clearly demonstrate that the total density of states (DOS), near the Fermi energy, is dominated by chain oxygen atoms. Expanding the YBC lattice along the c-axis shows an increase in the chain DOS which may account for the experimentally observed slight increase in T$_c$ for Au doped YBC.

## 1.    Introduction

Despite well over 30,000 technical publications concerning high temperature superconductors, a consensus regarding the pairing mechanism is yet to emerge. Two very different theoretical views have recently received prominence, namely pairing mechanisms based upon 'spin fluctuations' [1] and 'Jahn-Teller polarons' [2]. In the view of the former, Cooper pairs result because of a felicitous disturbance in the lattice's spin pattern as an electron propagates through the material. In the latter, the crystal spontaneously distorts to remove ground state degeneracy and in doing so locally polarises the lattice. Such 'polarons' (electron plus local distortion) bind into Cooper pairs that persist at relatively high temperature.

Johnson et al. [3] suggests that the Jahn-Teller distortion of the lattice is coherently aided by phonons. An interesting consequence of this model is that the condensates, based upon oxygen (π-bonded) p-orbitals, are located *in the chains* of the cuprate superconductor YBC. 'π-Bonded' tubes that run along the a-axis, based upon O4 2p$_y$ orbitals are evident in the charge density calculations of Pickett et al. [4]. Among the plethora of high T$_c$ models, Johnson's is the only one as far as we are aware, that assumes the condensates originate in the chains or 'charge reservoir'. Given the role assumed for phonons in Johnson's model, T$_c$ should depend on the DOS. Furthermore the carriers behave like a particle in a box, changing the confinement (i. e. lattice parameter) changes the DOS.

The notion of chain based superconductivity is supported by the compelling work of Dow and Harshman [5]. They demonstrate convincingly that the superconducting condensates in YBC and its homologues reside in the chains, specifically in the Ba-apical oxygen (O4) YBC layer. This is in stark contrast to the widely held view that such condensates reside in the CuO$_2$ layers of this material.

## 2.    Method of Calculation

We have investigated the possible role of oxygen chain sites in the superconductivity of YBC by calculating the oxygen partial DOS, using the WIEN2K ab initio crystal properties computer suite [6]. The calculations are performed in the density functional picture using the generalized gradient approximation with the LAPW + lo method. They allow the identification of electronic structure with atomic orbitals.

The YBC lattice parameters used are those determined by Cieplak et al. [7] using x-ray and neutron diffraction. The calculation is repeated with and without an expanded c-axis. The c-axis is chosen since this axis expands in Au doped YBC [7]. The expansion however is not uniform with most of the expansion occurring between O4 atoms. This represents the distance between π-bonded tubes in Johnson's model. As a first step we choose an expansion equal to

2 % along the c-axis. The unit cell of orthorhombic YBC with alternating chain sites fully occupied by oxygen atoms (ortho I) is shown in Fig.1.
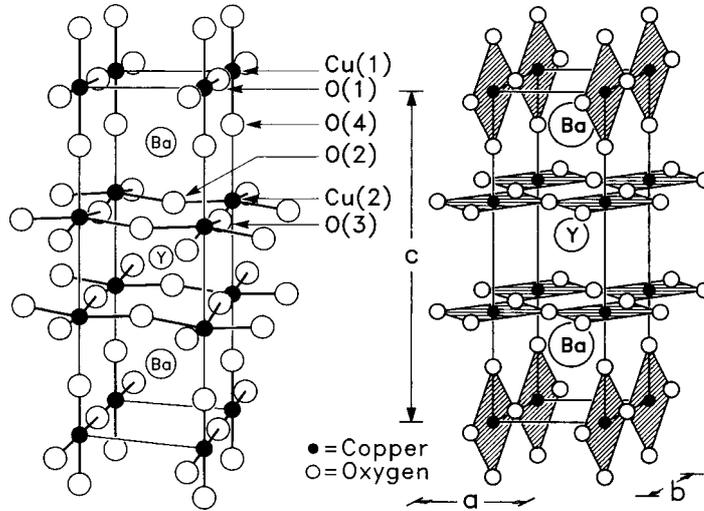


Fig. 1. Orthorhombic structure [8] of YBC with Cu and O sites designated. Right figure distinguishes planes (horizontal diamonds) from the 'charge reservoir' (vertical diamonds).

## 3.    Results and Discussion

The total DOS and individual DOS for the two copper sites Cu1 and Cu2 together with chain and plane oxygens are shown in Figs 2, 3, 4 and 5 for the experimentally observed YBC lattice. The calculation clearly shows that the chain oxygen atoms dominate the total DOS at the Fermi level ( = 0 eV). In what follows we therefore focus our attention on the chain oxygen DOS and in particular O4 (2p) since it plays a central role in Johnson's model. The partial O4 (2p) DOS for the experimental and 2 % expanded YBC lattice is shown in Fig.6. This shows a noticeable increase in DOS at the Fermi level with increase in lattice parameter.
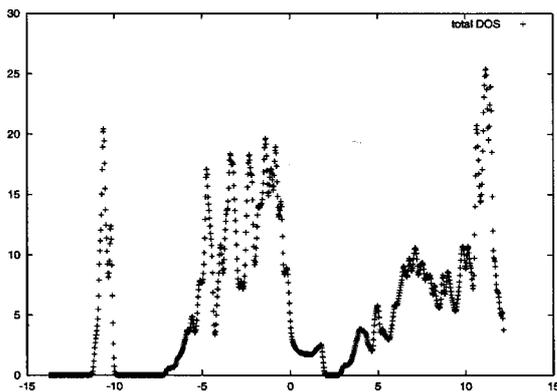


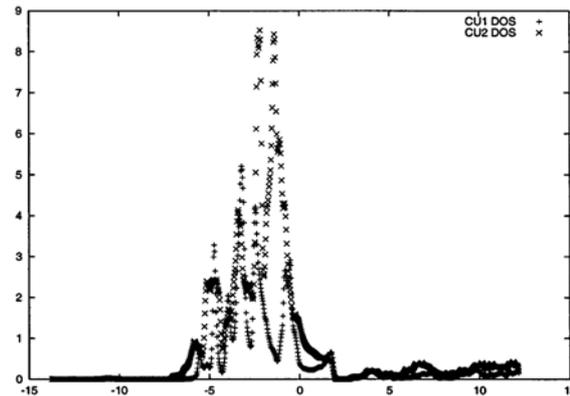Fig. 2. Total DOS versus energy in eV.

Fig. 3. Comparison of Cu1, Cu2 sites total DOS versus energy in eV.
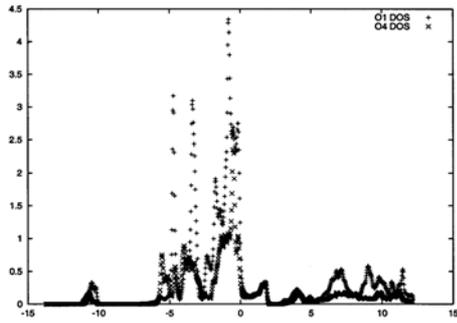
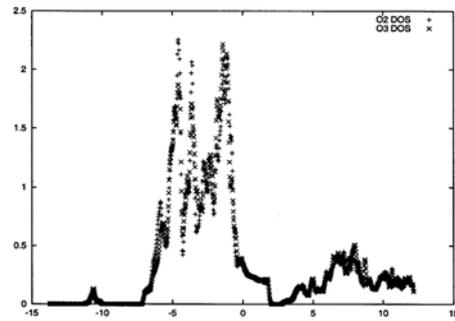Fig. 4. Comparison of O1, O4 sites total DOS versus energy in eV.



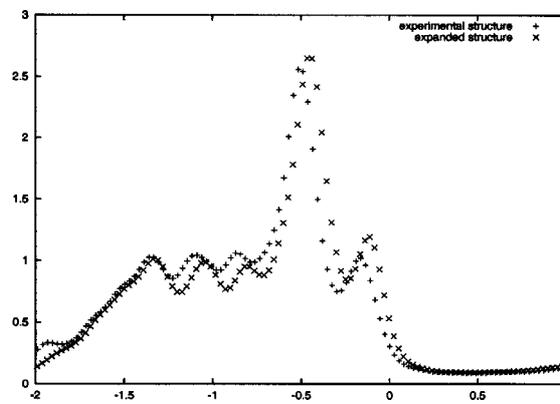Fig. 5. Comparison of O2, O3 sites total DOS versus energy in eV.



Fig. 6. Comparison of partial 2p DOS for O4 site
for different crystal structures versus energy in eV.

Cieplak et al. [7] explained an observed slight increase in $T_c$ with gold doping, as simply a hole doping effect. Since gold is known to draw additional oxygen ($\delta \sim 7.04$) into YBC at interstitial O5 sites it was assumed that additional holes were doped into the planes which were *assumed* to be superconducting. The work of Dow and Harshman (and references therein) shows that this cannot be the case. The present work, inspired by Johnson's real space molecular orbital approach, suggests that the enhancement may be due to a slight increase in the O4 (2p) partial DOS. If this suggestion ultimately proves to be true, then phonons may play a significant role in the cuprates.

**References**
[1]    D. J. Scalapino, *J. Phys. Chem. Solids*, **54**, 1433 (1993).
[2]    G. Zhao, M. B. Hunt, H. Keller and K. A. Muller, *Nature*, **385**, 236 (1997).
[3]    K. H. Johnson, D. P. Clougherty and M. E. McHenry, *Mod. Phys. Lett.*, **B3**, 1367 (1989).
[4]    W. E. Pickett, *Rev. Mod. Phys.*, **61**, 433 (1989).
[5]    J. D. Dow and D. R. Harshman, *Phil. Mag.B*, **82**, 1055 (2002).
[6]    P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicak and J. Luita, *WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties* (Karlheinz Schwarz, Techn. Universität Wien, Austria, 2001).
[7]    M. Z. Cieplak, G. Xiao, C. L. Chien, A. Bakhshai, D. Artymowicz, W. Bryden, J. K. Stalick and J. J. Rhyne, Phys. Rev. B, **42**, 6200 (1990).
[8]    R. Beyers and T.M. Shaw, Solid State Physics, **42,** 135 (1989).