Self Consistent Field, SCF HOMO and LUMO for CuO2 Layer in Cuprates

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**ABSTRACT:**

Before photoemission studies [1995] measured the symmetry of layer cuprate conduction states along the (xy), (x-y) direction of the unit cell, a SCF analysis [1993] gave the symmetry of the HOMO & LUMO showing O2p\(_x\)-O2p\(_y\) charge de-localization for the conducting CuO\(_2\) layer in a superconducting cuprate (T=Nd\(_2\)CuO\(_4\) in the crystal field of point charges of nearest neighbor unit cells). The predictive power of MO calculations are applied now to understand the concept of valence and periodic lattice distortions commonly found in these solids [2003].

1. The Approach:

The conducting (CuO\(_4\))\(^{2-}\) layer in superconducting cuprates may be represented as a negatively charged covalent metallic sheet balanced by a field of counter charges +Q in the lattice, i.e., the metallic sheet is intercalated between ionic charges (Fig.1). Self consistent field SCF calculations [1993] provide the symmetry of the basis HOMO & LUMO: Cu\(^{2+}\) and Cu\(^{3+}\) MO in ~nm\(^2\) CELL. Doubly degenerate Cu4O4 MO give 5\(^{th}\) degeneracy for i = 53, etc. (Fig. 2) and i' = 107. Electrons along the \(\pm \pi\) & \(-\pi\) diagonals contribute to transport properties.

2. Calculation of structural properties in superconducting cuprate films:

The advantage of an MO over a band structure calculation lies on the fact that the MO give directly the bond overlap charge, which in turn determines the de-localized charge. The overlap charge in the M-M' bond is determined by the occupied states i which are a superposition of atomic orbitals \(\phi_i\) centered at \(R_i\). The MO given by programs MOTEC/METTEC/MOLECOLE [1991], developed by E. Clementi and G. Corongiu using a LINUX PC, obtain the bond overlap population, \(\Omega_{\text{M-M'}}\): (1)

\[
\Omega_{\text{M-M'}} = \sum_i \psi_i^*(R_{i-M}) \phi_i(R_M) \psi_i(R_{i-M'}) \phi_i^*(R_M')
\]

The atomic number Z minus the gross population is:

\[
V_M = Z_M - \Omega_{\text{M-M'}}
\]

The overlap population in benzene/graphite, independent of \(V_O\) compression part of the PLD and decreases on the expansion side of the wave due to charge repulsion.

3. RESULTS, DISCUSSION

**SUMMARY:** The (CuO\(_2\))\(^{2-}\) layer of a cuprate nano-particle may be described by covalent bonds.

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- \(V_M\) = Mulliken M Gross electron population. (3)

4. Conclusions:

The overlap charge along O2p\(_{x}\)-O2p\(_{y}\) direction remains at 0.5 electron charge only half of the C-C overlap population in benzene/graphite, independent of \(V_O\) = -1.3. The inner de-localized electron overlap Cu-O charge along the a-axis depends strongly on \(V_C\) and approaches zero as \(V_C\) \(\rightarrow\) +2. PLD are allowed because \(\Delta E_{\text{PLD}}\) \(\approx\) \(\Delta E_{\text{LUMO}}\). The energy is higher in the compression part of the PLD and decreases on the expansion side of the wave due to charge repulsion. In Q is very important.