Utilization of a Highly Correlated Cluster Model for Interpretation of Electronic Spectroscopic Data for The High-Temperature Superconductors

By

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Utilization of a Highly Correlated Cluster Model for Interpretation of Electronic Spectroscopic Data for the High-Temperature Superconductor.

We have consistently interpreted electron spectroscopic data for the high temperature superconductors utilizing a highly-correlated CuO$_7$ cluster model, and an extended Hubbard Hamiltonian which includes the inter-site Cu-O and U-U parameters. The data indicate much larger U$_{pp}$ and U$_{pp}$ values than found in other typical highly conductive metals. Previously unassigned features in the data are now assigned within the model.
UTILIZATION OF A HIGHLY-CORRELATED CuO₆ CLUSTER MODEL TO INTERPRET ELECTRON SPECTROSCOPIC DATA FOR THE HIGH-TEMPERATURE SUPERCONDUCTORS

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ABSTRACT

We have consistently interpreted electron spectroscopic data for the high temperature superconductors utilizing a highly-correlated CuO₆ cluster model, and an extended Hubbard Hamiltonian which includes the inter-site Cu-O Uₑ and O-O Uₚ parameters. The data indicate much larger Uₑ and Uₚ values than found in other typical highly conductive metals. Previously unassigned features in the data are now assigned within the model.

INTRODUCTION

In this work we summarize results of an interpretation of electron spectroscopic data for the high temperature superconductors. The data interpreted include the valence band (VB), Cu 2p, and O 1s photoelectron data (UPS and XPS), the Cu L₃,M₅, Vu and O KVV Auger data, and the O K and Cu L₃ x-ray absorption and emission (XANES and XES) data. Published data for polycrystalline and single crystal samples of La₂₋ₓBaₓCuO₄ and YBa₂Cu₃O₆₋ₓ (herein referred to as the La and 123 HTSC's) are considered along with that for CuO and Cu₂O. The basic electronic structure of the HTSC's can be described with the Anderson Hamiltonian utilized by Sawatzky and coworkers. It includes the transfer or hopping integral t, the Cu and O orbital energies eₐ and eₚ, the core polarization energy Qₐ, and the intra-site Coulomb repulsion energies Uₑ and Uₚ (the latter sometimes are assumed to be zero). This model is most useful when the U's are large relative to the band width, i.e., when correlation effects dominate hybridization effects. A CuO₆(Cu₁₋ₓ₋ₓ) cluster model, which is also reasonably valid when U >> t, simplifies the model further. We utilize an extended Hubbard model by adding the inter-site repulsion energies Uₑ and Uₚ (i.e., between neighboring Cu-O and O-O atoms). The addition of these interactions is important for understanding many of the features in the data.

RESULTS

Our results for the Hubbard parameters are summarized at the top of Table 1. Other estimates of these Hubbard U and ε parameters have been reported previously for the HTSC's. These were obtained empirically from the Cu 2p XPS and the VB UPS data utilizing the Anderson model. Our optimal extended Hubbard

*Supported in part by the Office of Naval Research.
results indicate that $U_{pp} = 12$ and $U_{pp}^* = 4.5$ eV for 123. These are much larger than previously thought for these metallic systems, although $U_{pp} - U_{pp}^*$ is in agreement with the best theoretical results above.

An upper estimate of the two-center $pp^*$ hole-hole repulsion, $U_{pp}^*$, can be obtained from the Klopman approximation,

$$U_{pp} = \frac{e^2}{r_{Cu}} + \frac{(2e^*/(U_{pp} + U_{pp}^*))^{1/2}},$$

where $r_{Cu}$ is the interatomic distance and $U_{pp}$ and $U_{pp}^*$ are the corresponding intra-atomic repulsion energies. Equation 1 gives a value for $U_{pp}^*$ around 4.5 eV assuming $r_{Cu} = 1.9$ Å. The large reduction in $U_{pp}$ may result from charge transfer into the Cu 4p levels to screen the Cu-O holes. Although metallic screening, which results from virtual electron-hole ($e-p$) pair excitations at the Fermi level, is not expected to be large in an insulator such as CuO, screening effects are expected to be much larger in metals, such as the HTSC's. The above results show that $U_{pp}$ is significantly reduced in both, and $U_{pp}^*$ remains large in both. The lack of a significant change in the $U$'s between CuO and the HTSC's indicates that the DOS at the Fermi level in the HTSC's must be very small.

Table 1 also correlates the calculated energies of the excited states with features in the experimental data. The CuO$_{n}$(v=1) cluster has one hole shared between the Cu 3d and O 2p shells in the ground state, which we term the $v$ (valence) states. The spectroscopic final states reflect multi-hole states, e.g. $v_1$, $v_2c$ (core) etc. The $v$ states, as reflected by the theoretical DOS, have the Cu-O bonding ($\sigma_+$) and antibonding ($\sigma_-$) orbitals centered at 4 and 0 eV, respectively, and the nonbonding Cu and O orbitals at 2 eV. The O features each have a width $2\Gamma = 4$ eV due to the O-O bonding and antibonding character and the Cu-O dispersion. We also define the Cu-O hybridization shift $\epsilon_0 = (\epsilon_0 + \epsilon_0^{Cu})/2$ and the Cu-O dispersion shift $\Delta$, which is utilized in Table 1 to give the energies. Thus, the ground state of an average CuO$_{n}$ cluster is located at 1 eV having the energy $\epsilon_0 - \epsilon_0^{Cu} = 0$, which we use as a reference energy for the excited states. In CuO, the hybridization shift $\Gamma$ is smaller, and we shall see below that $\Delta_{CuO-Cu}$ has increased to 1 eV.

Those clusters containing additional charge carrier holes (these exist in doped La, and 123 when $x > 0.5$) actually have two holes per CuO$_{n}$ cluster. The average $v^*$ ground state, which is dominated by the $pp^*$ configuration, i.e. the charge carrier holes spend most of their time on the O atoms, so we indicate this ground state by the
TABLE 1 Summary of hole states revealed in the spectroscopic data, and estimated energies using the following optimal values for the Hubbard parameters in eV:

\[ \delta_1 = 2 \quad \epsilon_z = 2 \quad U_p = 12, 13 \quad U_d = 9.5, 10.2 \]
\[ \delta_2 = 0.5, 0.8 \quad \epsilon_z = 2, 3 \quad U_{p*} = 4.5, 4 \quad U_{d*} = 2 \]
\[ \epsilon = 1, 0.5 \quad \delta = 2 \quad \Delta = 0, 1. \quad \kappa = 4 \]

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<tr>
<th>State</th>
<th>Energy expression</th>
<th>Calc. E. eV</th>
<th>Exp. E. eV</th>
<th>Remark</th>
</tr>
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<td>G.S. and IPES, w</td>
<td>$\epsilon_z - \delta_1 + \Gamma$</td>
<td>0 $\neq$ 2</td>
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<td>UPS and XES, v</td>
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<td>2.5</td>
<td>2.5</td>
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<td></td>
<td>$\epsilon_z + U_{p*} + \delta_1 + \alpha$</td>
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<td>4.2</td>
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<td></td>
<td>$\epsilon_z + \Delta + U_{p*} + \delta_1 + \alpha$</td>
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<td></td>
<td>$\epsilon_z + \Delta + U_{p*} + \delta_1 + \alpha$</td>
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<td>9.5</td>
<td>mystery peak</td>
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<td>Cu 2p XPS, cv</td>
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<td>12.5</td>
<td>Cu saturation</td>
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<tr>
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<td>$\epsilon_{1+4.5}$</td>
<td>?</td>
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<td>$\epsilon_{1+14}$</td>
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<td>$\epsilon_z + 1$</td>
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<td>no mix</td>
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<td>15.5</td>
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### TABLE 1 (cont.)

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<th>State†</th>
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<th>Exp. E. E.</th>
<th>Remark</th>
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<td>$e_v + 9$</td>
<td>$E_2p + 10$</td>
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<td>dcp</td>
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<td>$e_v + 17$</td>
<td>$E_2p + 18$</td>
<td>main, L</td>
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<td>cp</td>
<td>$e_v + \alpha$</td>
<td>$e_v + 15$</td>
<td>-</td>
<td>not</td>
</tr>
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<td>cd</td>
<td>$e_v + 2\alpha$</td>
<td>$e_v + 30.5$</td>
<td>-</td>
<td>obs.</td>
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<td></td>
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<td>d = c</td>
<td>$e_v - e_v + \delta_1$</td>
<td>$E_{1s} - 1$</td>
<td>$E_{1s} - 1.4$</td>
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<td>$E_{1s} - CB$</td>
<td>$E_{1s} + 1.2$</td>
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<td>pp² = cp</td>
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<td>$E_{1s}$</td>
<td>middle</td>
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<tr>
<td>O K KELLS, c</td>
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<td></td>
</tr>
<tr>
<td>d = c</td>
<td>$e_v - e_v + \delta_1$</td>
<td>$E_{1s} - 1$</td>
<td>$E_{1s}$</td>
<td>edge</td>
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<tr>
<td>cdCB</td>
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<td>$E_{1s} - CB$</td>
<td>$E_{1s} + 1.7$</td>
<td>upper</td>
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<tr>
<td>pp² = cd</td>
<td>$e_v - 2\alpha - e_v + \delta_1 + \delta_3 + \delta_4$</td>
<td>$E_{1s} - 0.5$</td>
<td>-</td>
<td>not obs</td>
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</table>

*Parameters for 123 indicated first, those for CuO second.  
†The calculated E is defined relative to the ground state $e_v$ (d), and the $e_v$ (pp²) ground state energy is $2e_v - \Delta$. The $v'(d)$ energy determines the Fermi level relative to the vacuum level at zero.  
*The dominant character switches as described in the text, and thus the sign in front of $\delta_1$ is the opposite for CuO.

The parameters in Table 1 were obtained by considering this same data plus XANES, Auger and XES data. Although we are in general agreement with the reported magnitudes for most of the parameters, our $U$ value is larger by about 2-3 eV so that it is consistent with the AES data. In Table 1, we indicate the location of two valence holes by d (Cu 3d) or p (O 2p). In the case of two holes on the oxygens, we distinguish two holes on the same O (p'), on ortho neighboring O atoms (pp'), or on para O atoms (pp̅') of the cluster. Furthermore, neighboring pp holes can dimerize, so we distinguish between two holes in bonded (pp') and antibonded (pp̅') O pairs. The magnitudes of the $U$ parameters are critical to the mechanism for the superconductivity. As a consequence, much effort has also gone into theoretically calculating these parameters, but wide disagreement still exists over the magnitudes. Theoretical values for $U$ in the range 6.5-10 eV, $U_p$ (actually $U_p - U_{pp}$) in the range 7-14 eV, and $U_{pp}$ in the range 0.6-1.6 eV have been reported, with the smaller results favored based on the quality of the calculations. No results for $U_{pp'}$ have been reported. Our empirical
notation p+. We use $2e^{-4}$-d as the energy of the p+ ground state relative to the vacuum level, where $a = 2$ eV is the energy shift between the principal p+ UPS final state at 2.5 eV and the lowest ground p+ states around 0.5 eV from the Fermi level.

The correlation between the calculated energies and experimental features, utilizing the indicated optimal Hubbard parameters, is very good. Details of this work are published elsewhere. Figs. 1 and 2 show examples of the UPS and Cu AES data for 123 and CuO, which reveal some of the features itemized in Table 1; the remaining data are published elsewhere.

![Figure 1](image1.png)  
Figure 1. Comparison of UPS spectra for CuO and 123 taken with the indicated photon energies in eV. Data for CuO from Ref. 10 (hv = 1487), 11 (hv = 74) and 12 (hv = 21). Data for 123 from Ref. 13 (hv = 25 and 74) and 14 (hv = 1487).

![Figure 2](image2.png)  
Figure 2. Comparison of Auger data for the materials indicated. $L_2M_4$ data for CuO and 123 from Ref. 15. $L_2M_4M_2$ data for CuO from Ref. 16 and for 123 from Ref. 9. The $L_2M_4$ data is on a 2-hole binding energy scale $E_2 = E_{12} + E_a$, and the $L_2M_4M_2$ data on a 1-hole scale $E_1 = E_{12} - E_a$, where $E_{12} = 935.4$ and $E_a = 77.3$ eV.

SUMMARY AND CONCLUSIONS

This work has allowed us to assign some previously unassigned features in the data, and greatly increased our understanding of the...
dynamical electronic processes which produce these features. We itemize our conclusions as follows:

1) A switch in the character of state 1 (see Table 1) from more dp to pp and vice versa for state 2 between CuO and 123 arises because \( \Delta \) decreases from 1 eV to 0 eV. The smaller \( \Delta \) in 123, due to a smaller \( \epsilon_p \) polarization energy, is consistent with the Cu 2p XPS and XES data (the latter showing this effect dramatically). Since state 1 is more of pp character in the SC's, the "charge carrier holes" (present in the La after Sr doping and in the 123 when \( 7-x \) is greater than 6.5) spend more time on the oxygens in 123 than in CuO.

2) The pp state is believed to be responsible for the "mystery" peak found at 9.5 eV in the UPS. Figure 1 indicates that such a peak also appears for CuO. This feature does not appear for CuO, as expected since UPS reflects the one-hole DOS in CuO. The smaller \( \Delta \) in CuO, due to a smaller \( \epsilon_p \) polarization energy, is consistent with the Cu 2p XPS and XES data (the latter showing this effect dramatically). Since state 1 is more of pp character in the SC's, the "charge carrier holes" spend more time on the oxygens in 123 than in CuO.

3) Although CuO, CuO, and NaCuO have a formal Cu valence of +1, +2, and +3, in the current picture they reflect the core DOS, with \( n_0 \), 1, and 2. Furthermore, we consistently predict the "chemical shifts" in the primary Cu 2p XPS peaks. Whereas, CuO exhibits just a primary core hole state at energy \( \epsilon_c \), CuO has its primary cd feature energy shifted by \( \Delta \epsilon_c \) relative to \( \epsilon_c \), and the primary cpp feature for NaCuO by \( \epsilon_c + \Delta \epsilon_c \) (Table 1), which is consistent with the experimental data. The width of the primary feature is seen to correlate with the intensity of the satellite, and is not due to the 0 p band width as suggested by others.

4) The increased "satellite" feature at 19 eV in the Cu LuVV Auger line shape for the HTSC's compared with CuO (see Fig. 2) arises because of increased final-state configuration mixing between the dp and dp states. Its intensity is increased in 123 relative to CuO because the energy separation (before hybridization) between dp and dp has decreased from 3.8 eV in CuO to 2.5 eV in 123. We have indicated this mixing in Table 1 by adding the hybridization shifts \( \Delta \) to the energy expressions for these two states.

5) We find that the initial-core shakeup (ICSU) process, which is known to be responsible for the satellite features in the Cu 2p XPS data, does not produce satellites in the AES or XES data, because the ICSU states generally "relax" to the primary states of the same symmetry before the core level decay. Such a relaxation is expected when the ICSU excitation energy is larger than the core level width. Previously, vanderLean et al., for the Cu halides, suggested that the intensity of these ICSU states in the XPS should be quantitatively reflected in the intensity of the Auger satellites found in the LuVV lineshapes. The data do not indicate this however. We previously suggested that a fraction of these ICSU states probably resulted in Auger satellites for the HTSC's, and that this fraction becomes larger as the covalency of the HTSC material increases. This work indicates rather that the ICSU states relax before the core level decay to states of the same symmetry, provided they have a ICSU excitation energy that is much greater.
than the core level width. We believe this to be a general result, at least in the Cu\textsuperscript{1+} materials.

6) The EELS and XANES data\textsuperscript{25-27} reflect the contributions from three possible transitions; the dominant d - c contribution nearest the Fermi level, the pps - cv (v = d or p) contribution resulting from the carrier hole states, as well as the cvCB contribution well above the Fermi level\textsuperscript{28}. Here CB represents an electron present in the higher Cu 4sp or O 3p "conduction band." The latter two contributions are not always resolved, and sometimes have been confused in the literature\textsuperscript{29-31}.

7) All of the temperature effects seen in the spectroscopic data\textsuperscript{32-35} can be attributed to a single phenomenon, namely a decrease in $\varepsilon_p$ due to increased metallic screening, or long range polarization. This is consistent with the decrease in the primary cp peak energy in the Cu 2p XPS, while the cd satellite remains unshifted. The larger energy separation between the cd and cp states decreases the mixing which causes the satellite to decrease in intensity and the main peak to get narrower. Although the primary cd peak does not shift in the O 1s XPS, a slight shift to lower energy is seen in the cp$^*$ and cp$^*$ contributions at lower temperature, as expected with a decrease in $\varepsilon_p$. The UPS spectra show a skewing toward the Fermi level at lower temperature, as expected with a decrease in $\varepsilon_p$. Finally the growth of the satellite intensity in the Cu L\textsubscript{2,3} Auger lineshape is consistent with a decrease in $\varepsilon_p$. The increased metallic like screening or polarization which appears to occur at lower temperature, reducing $\varepsilon_p$, probably involves the grain boundaries, since the more recent data for the single crystal samples do not change with temperature\textsuperscript{36}.

In summary, an interpretation of the data utilizing a highly correlated CuO\textsubscript{1+} cluster model shows that a single set of Hubbard parameters predicts all of the state energies. Changes in the data between CuO and the HTSC's arises primarily from a reduction in $\varepsilon_p$; this reduction continues with decreasing temperature in the HTSC's due to increased metallic screening. Compared with CuO, the HTSC's show an increased covalent interaction between the Cu-O bonds. The large size of U$_p$, and the temperature dependence, reveal that metallic screening is incomplete, and hence that the DOS at the Fermi level in the HTSC's is relatively small.

REFERENCES

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