TIGHT-BINDING STUDY OF THE ELECTRONIC STRUCTURE OF THE HIGH TEMPERATURE SUPERCONDUCTOR La_2CuO_4

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ABSTRACT

We have fit our first principles LAPW band structure results for the high T_c superconductor La_2CuO_4 to a tight-binding Hamiltonian that contains s, p, and d interactions from the three components of these materials. Our fit reproduces very accurately the 17 lower bands of this material and especially the Fermi surface.

This year's discoveries of high temperature superconductors created a large number of investigations to understand the mechanism responsible for this new phenomenon. Many of the theories proposed are based on tight-binding Hamiltonians (TBH) of varying complexity. In this work we present the results of a Slater-Koster (SK) fit to our first principles band structure calculation [1] for La_2CuO_4. Other authors [2,3] have reported tight-binding parametrizations of the band structure of La_2CuO_4 which claim that they reproduce the LAPW results well. The calculation of the La_2CuO_4 phonon spectrum by Weber [2] is based on a non-orthogonal TBH fit to the LAPW calculation of Mattheiss [4]. Weber has used a 27-orbital basis, but gives no information about the quality of his fit, and presents no figure of the energy bands so that the reader can assess the accuracy of his calculation. The calculation of Richert and Allen [3] is based on Harrison type SK parameters and reproduces only qualitative features of the band structure of this material. In this paper we wish to give details of our procedure which we believe to be of superior accuracy. We have used a 31x31 orthogonal TBH in the two-center approximation that includes La-d, Cu-s,p,d and O-p orbitals. This TBH requires 44 two-center parameters which are determined by fitting to our LAPW results at 71 k-points in the irreducible tetragonal Brillouin zone, including an energy range that spans a minimum of 17 to a maximum of 19 energy bands depending on the k-point. Our rms deviation from the first principles results is 14 mRy taken for the lower 17 bands and all the 71 k-points fitted. The 17th band which is the

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one determining the Fermi surface in this material is fitted with an rms error of 6 mRy. In the fitting of the LAPW energy eigenvalues we have minimized the following function for each eigenvalue:

$$F = (E_{LAPW}-E_{SK})^2 + \frac{1}{4}\ (Q_{LAPW}-Q_{SK})^2 \qquad (1)$$

where E are the eigenvalues and Q the electronic charges of each atom site for all angular momentum components. The inclusion of the second term in Eq. 1 is essential in materials with complicated crystal structures in order to preserve the angular momentum character of the various states involved and to avoid switching of the ordering of energy levels.

Our resulting SK energy bands are compared to the LAPW bands in panels (a) and (b) of Fig. 1. We note that near the Fermi level E_F, we have excellent agreement between LAPW and SK. The respective E_F values coincide to within 1 mRy and the energy bands near E_F look almost identical in all directions. Some discrepancies between the two approaches are found in the lower bands. It is interesting to note that an inspection of our on-site SK parameters reveals that the O_z p-state energy is almost identical to the average Cu-d on-site energy. The O_{xy} p-state energy is found to be approximately 60 mRy below the O_z. The difference between the two O sites is usually discussed in terms of Jahn-Teller distortion. A similar comparison of the densities of states is given in Fig. 2. It is important to note that the van Hove singularity just below E_F is found in the SK results as well. This peak has been suggested [1] to be responsible for the enhancement of the superconducting temperature upon doping with Ba or Sr. Therefore our TB Hamiltonian seems to be at the level of accuracy required to deal with the problems of rare earth substitutions as well as oxygen vacancies. In subsequent paper we will address these questions using the coherent potential approximation method.

ACKNOWLEDGEMENTS

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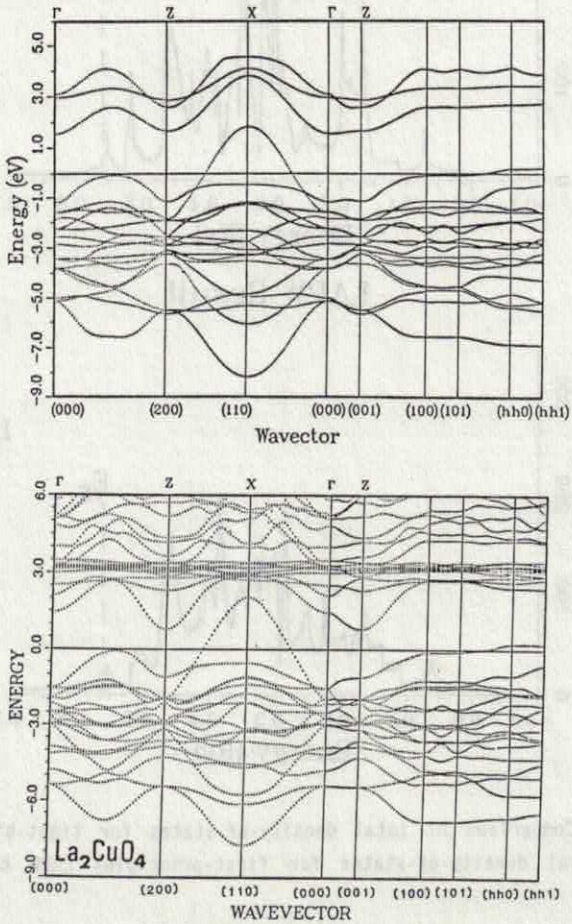

Figure 1. Comparison of La_2CuO_4 energy bands calculated from tight-binding fit (top) to those from first-principles LAPW calculation (bottom). For clarity, only the lowest twenty tight-binding bands are shown.

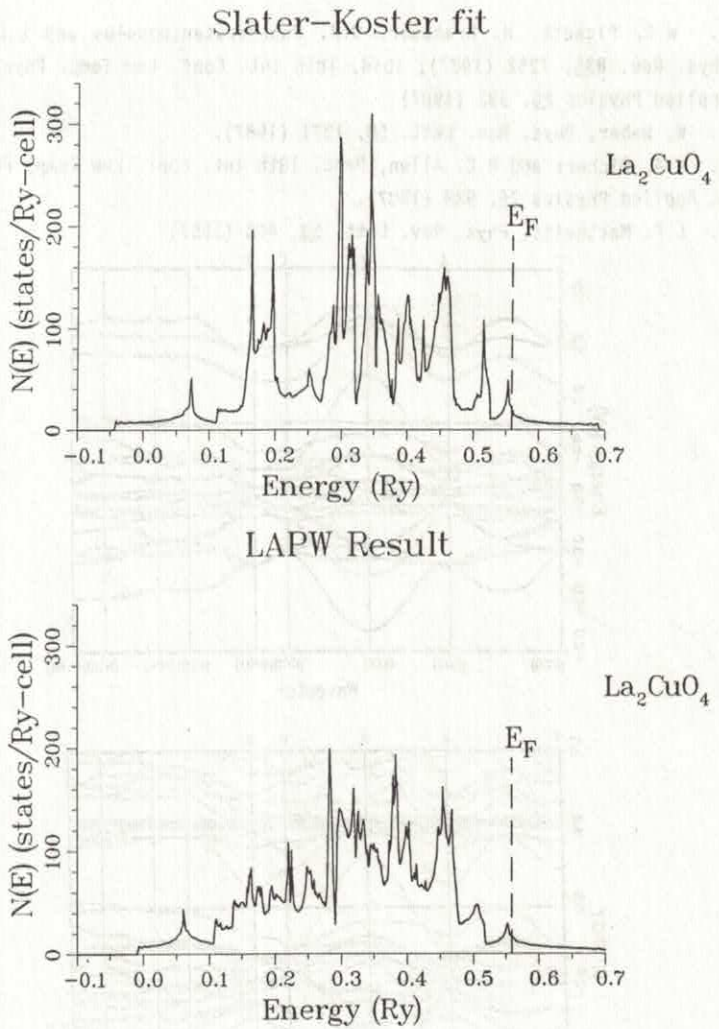

Figure 2. Comparison of total density-of-states for tight-binding fit (top) to total density-of-states for first-principles LAPW calculation (bottom).