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Orbital distribution of holes in the linear chain cuprate Sr_2CuO_3

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The electronic structure of the prototypical linear chain cuprate Sr_2CuO_3 is studied theoretically by exact diagonalizations (ED) for clusters within the framework of generalized *pd*-models as well as by bandstructure calculations. From the 4- and 7-band analysis of the Sr_2CuO_3 band structure, enhanced values of Cu-O transfer integrals have been derived. The results are compared with polarization dependent O 1*s* x-ray absorption spectroscopy measurements (XAS) [1]. From the observed anisotropy of the XAS intensities significantly enhanced values of the intersite Coulomb interactions V_{pd} and V_{dd} compared with typical layered cuprates can be deduced.
Keywords: Electronic structure, Intersite Coulomb interaction, One-dimensional cuprates,

1. INTRODUCTION

Sr_2CuO_3 is the best known realization of a spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain, [2] showing what is possibly a record value for the nearest neighbor (n.n.) exchange parameter $J \approx$ 200 to 260 meV, which significantly exceeds the corresponding values in the 2D cuprates of 130 to 150 meV. The origin for this unexpected high J value remains unclear and its elucidation requires a detailed knowledge of the underlying electronic structure. It is the aim of our analysis to contribute to the understanding of these chains and to propose a possible scenario of the large J.

2. MODEL

Starting from a detailed multi-band analysis of LDA-LCAO band structure calculations, we show which orbitals are mainly involved in low energy excitations and yield insight in the magnitude of the corresponding transfer integrals. We shall describe the chain cuprates under consideration by the extended 4-band *dp* Hubbard-model written within standard notation (see also Fig. 1):

$$H = \sum_i \varepsilon_i \hat{n}_i + \sum_{<i,j>,s} t_{ij}(c^\dagger_{i,s} c_{j,s} + \text{H.C.}) + \sum_i U_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \sum_{<i,j>} V_{ij}\hat{n}_i\hat{n}_j. \quad (1)$$

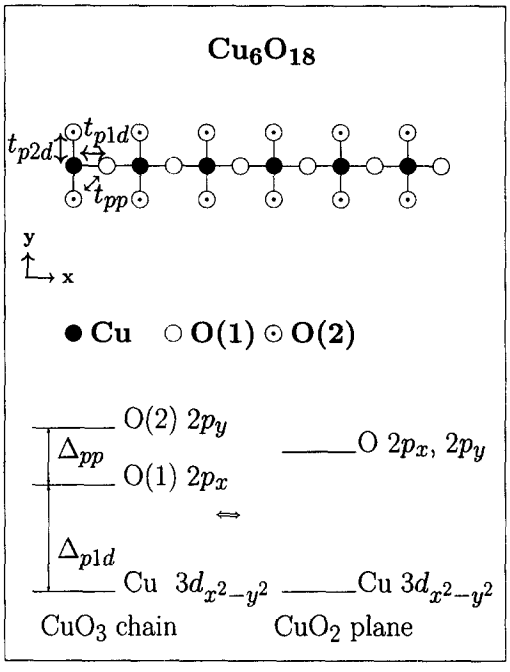

Figure 1. Sketch of the cluster modeling the CuO_3 chains in Sr_2CuO_3 within the *pd*-Hamiltonian (Eq. (1)) adopted. Upper half: The periodic clusters considered here. Lower half: On-site energies for the two inequivalent oxygen sites.

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3. RESULTS AND DISCUSSION

According to the orbital analysis [3] three orbitals contribute more than 94 % to the total density of states of the antibonding band, namely the O(1) $2p_x$ and O(2) $2p_y$ as well as the Cu $3d_{x^2-y^2}$ states. Hence, the usual *pd*-model with one orbital per site but extended to two nonequivalent oxygen sites per unit cell is a good first approximation. Our LDA-LCAO transfer integrals derived from a 7-band fit [3] read: $t_{p1d} = 1.57\text{eV}, t_{p2d} = 1.8\text{eV}, t_{pp} = 0.62eV$. We regard them as a reasonable estimate (from above) of the hopping parameters which enter Eq. (1).

Calculating with the aid of exact diagonalizations and Monte Carlo calculations the occupation numbers n_{pi} at the O(i) sites i=1,2 changing systematically the most unknown Hamiltonian parameters Δ_{pp} and V_{pd}, we reproduced the experimental anisotropy of the XAS-intensities [1]

$$R = 2n_{p2}/n_{p1} = 1.22, \qquad (2)$$

as shown in Fig. 2. If reasonable values for $\Delta_{pp} \sim$ 0.5 to 0.75 eV are adopted, Eq. (2) can be satisfied , only if a significantly enhanced intersite Coulomb interaction V_{pd} (i.e. nearly twice as large as for typical layered cuprates) is admitted. From the strong excitonic effects seen in the EELS data [4], analyzed within an effective one-band extended Hubbard model, a large interplaquette Coulomb repulsion $V \approx 0.8$ eV has been deduced. Within our approach this points to the relevance of further n.n.n. interactions such as a weak Cu-Cu $V_{dd} \approx 0.85$ eV and $V_{pp} \approx 1.35$ to 1.5 eV.

To summarize, our analysis reveals strong support for the suggested enhanced intersite Coulomb interaction V_{pd} in Sr_2CuO_3 derived from the relatively small value $\Delta_{pd} \leq 3$eV to explain the Cu XPS data [5] although at somewhat larger transfer integrals in our case. The latter result might explain together with a sizeable ferromagnetic contribution to the total exchange parameter $J \approx 260$ meV its unusual large value.

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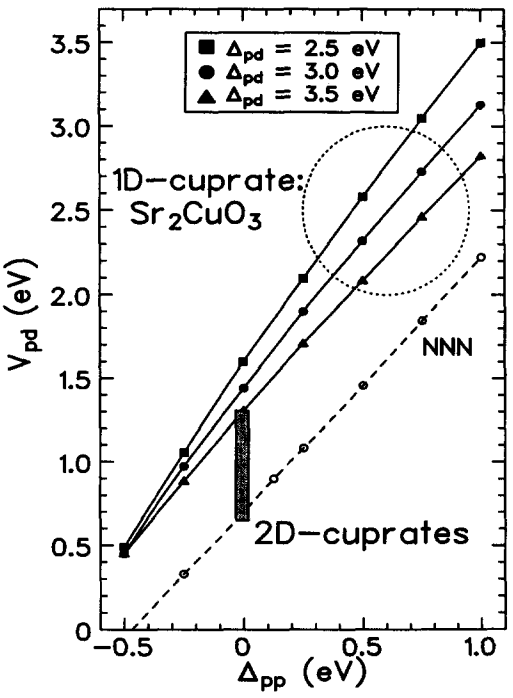

Figure 2. The obtained empirical relationship between the oxygen on-site energy difference Δ_{pp} and the intersite Coulomb interaction V_{pd} The curve denoted by 'NNN' has been obtained including next-nearest-neighbor Coulomb interaction. The circle and the box indicate the most favored parameter ranges for Sr_2CuO_3 and the 2D cuprates, respectively.

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