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Physica B 259–261 (1999) 1001–1002

PHYSICA B

The electronic structure of Li_2CuO_2

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Abstract

The band structure, the total and the partial densities of states have been calculated for Li_2CuO_2 within the local density approximation. The obtained metallic behaviour with one narrow antibonding band crossing the Fermi level is in sharp contrast with the observed insulating state resulting from strong electron correlations. Li_2CuO_2 is usually considered as the best realization for an one-dimensional (1D) edge-sharing CuO_2 chain, here we find instead a comparable dispersion in all three dimensions for the antibonding band. We compare the electronic structure of Li_2CuO_2 with that of really quasi-1D cuprates $Sr(Ca)_2CuO_3$, $SrCuO_2$, and $CuGeO_3$.

PACS: 74.72.Jt; 75.30.Gw

Keywords: Li_2CuO_2; Band structure calculation; Cuprates

Recently, quasi-one-dimensional (1D) cuprate compounds have been studied extensively. They are allowing theoretical and experimental access to a number of basic physical phenomena in low dimensions. In the undoped case, these materials are charge transfer insulators with a rich variety of magnetic properties. At low temperatures, they show phase transitions to an antiferromagnetic state in the corner-sharing CuO_3 single or Cu_2O_4 double chain ($Sr(Ca)_2CuO_3$ and $SrCuO_2$, respectively), to a spin Peierls phase in the edge-sharing CuO_2 chain of $CuGeO_3$ and to a ferromagnetic ordering along the analogous CuO_2 chain of the Li_2CuO_2 compound [1] considered in the present work.

Li_2CuO_2 exhibits a body centered orthorhombic structure with lattice constants $a = 2.860$ Å, $b = 9.377$ Å, and $c = 3.654$ Å [1], where the CuO_2 chains run in a direction. In order to get insight into the electronic structure of Li_2CuO_2 we have performed linear combination of atomic orbitals (LDA–LCAO) and linear muffin-tin orbital approximation (LMTO) band structure calculations with a minimum basis treating the Cu (4s, 4p, 3d) O (2s, 2p), and the Li (2s, 2p) orbitals as local valence basis states and the lower lying states as core states. Due to the relatively open crystal structure two empty spheres per unit cell have been introduced.

The total and the partial densities of states (DOS) are shown in Fig. 1. The sharp peak in the *center* of the antibonding band with nearly pure Cu 3d and O 2p character is in sharp contrast to remnants of 1D van Hove singularities near the band edges in the corresponding antibonding bands of $Sr(Ca)_2CuO_3$ [2] and $CuGeO_3$ [3] and gives strong evidence for a non quasi-1D electronic structure. More detailed investigations show that the peak at the Fermi level is composed mainly of Cu $3d_{xy}$ and O $2p_{x,y}$ states, with almost equal contributions from both O orbitals at variance to the above-mentioned corner-sharing CuO_3 chain compounds. The last circumstance provides a natural explanation for the observed ferromagnetic coupling in chain direction.

As expected from simple chemical considerations of the valence there is a single, half-filled, well separated antibonding band crossing the Fermi level (see Fig. 2). On the one hand, the width of this band is about 1 eV and similar to $CuGeO_3$, but on the other hand, its

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0921-4526/99/$ – see front matter
PII: S0921-4526(98)00687-5

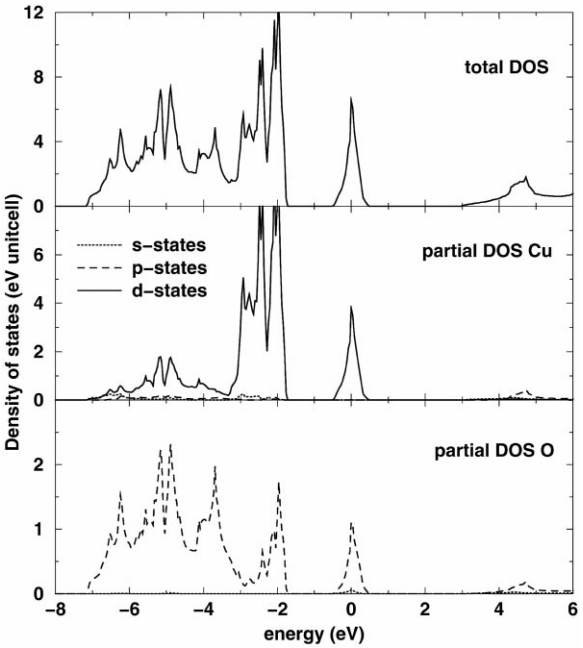

Fig. 1. Total and partial DOS of Li_2CuO_2 (Li not shown) with the Fermi level at zero energy.

dispersion in chain direction ((0, 0, 0) → (1, 0, 0)) exceeds the dispersion in the other two directions by a factor of two only. A strong effect of next nearest neighbour interactions in chain direction has been derived from a strong second harmonic contribution to the calculated dispersion. Important is the equivalence of the dispersion in the two transverse directions pointing to a specific interchain interaction. The moderate anisotropy (compared with the above mentioned cuprates) due to that interaction is in sharp contrast to the widely held intuitive view considering Li_2CuO_2 as the best realization of an 1D-edge-sharing CuO_2 chain [4]. Further consequences, details, and a comparison with available experimental data will be published elsewhere.

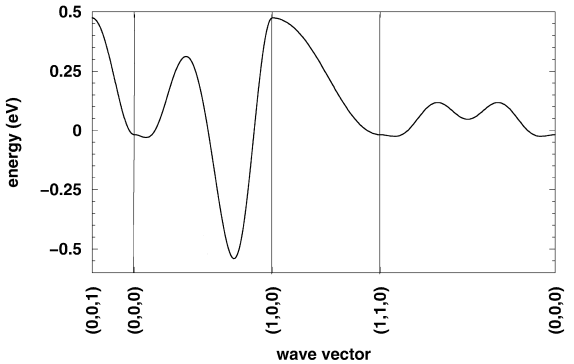

Fig. 2. The band dispersion of the antibonding band of Li_2CuO_2 along the main symmetry lines. The wavevector is given in units of $(\pi/a, \pi/b, \pi/c)$.

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