Electronic structure of La$_2$CuO$_4$

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MS received 22 June 1989

Abstract. The electronic band structure of La$_2$CuO$_4$ is performed using self-consistent linear muffin-tin orbital method. The 17 band complex is found to arise mainly from the overlap between Cu-3d and O-2p wavefunctions. The calculated density of states at the Fermi energy ($N(E_F)$), the conduction band-width and the electronic specific heat coefficient are given.

Keywords. Electronic structure; band structure; electronic specific heat coefficient.

PACS No. 71.25

In this paper we report the electron energy band structure of La$_2$CuO$_4$ performed using the self-consistent linear muffin tin orbital (LMTO) method. Results obtained are compared with the band structure calculations reported earlier (Mattheiss 1987; Yu et al 1987; Oguchi 1987; Fujiwara and Hatsugai 1987; Takegahara et al 1987 and Pickett et al 1987). The lattice constants corresponding to the bct phase of La$_2$CuO$_4$ and the sphere radii of the atoms are given in table 1 (Fujiwara and Hatsugai 1987; Takegahara et al 1987 and Takagi et al 1987).

The relativistic Hartee-Fock equation was used to generate the core and atomic charge densities to construct the potential parameters of the respective atoms for the initial run. We use Barth-Hedin exchange-correlation potential in the LMTO calculation (Andersen 1975; Skriver 1984). About 60 iterations were carried out to achieve the self-consistency and the eigenvalues were calculated to an accuracy of 1 mRyd. The band structure calculations were performed for 140 $k$-points. The band structure and the density of states histograms are given in figures 1 and 2. The bands obtained are very similar to that reported earlier (Mattheiss 1987; Yu et al 1987; Oguchi 1987; Fujiwara and Hatsugai 1987; Takegahara et al 1987 and Pickett et al

Table 1. Lattice constant and the sphere radii of La$_2$CuO$_4$ (in a.u.).

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<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>a</td>
<td>7.1464</td>
</tr>
<tr>
<td>c</td>
<td>25.0364</td>
</tr>
<tr>
<td>$S_{La}$</td>
<td>3.6504</td>
</tr>
<tr>
<td>$S_{Cu}$</td>
<td>2.6884</td>
</tr>
<tr>
<td>$S_{O1}$</td>
<td>2.1014</td>
</tr>
<tr>
<td>$S_{O2}$</td>
<td>2.1014</td>
</tr>
</tbody>
</table>
Figure 1. Energy bands of $\text{La}_2\text{CuO}_4$.

Figure 2. Density of states of $\text{La}_2\text{CuO}_4$. 
Table 2. Comparison of the density of states at \( E_F \) of the present work with the earlier works.

<table>
<thead>
<tr>
<th>( N(E_F) ) States/Ryd-formula unit</th>
<th>Partial density of states (States/Ryd-formula unit)</th>
<th>Conduction band-width (Ryd.)</th>
<th>( \gamma ) (mJ/mol K(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present work</td>
<td>La 21.474 Cu 0.415 Ox1 12.006 Ox2 3.215 1.346</td>
<td>LMTO</td>
<td>0.5208</td>
</tr>
<tr>
<td>Oguchi</td>
<td></td>
<td>LMTO</td>
<td></td>
</tr>
<tr>
<td>Takegahara</td>
<td></td>
<td>APW</td>
<td></td>
</tr>
<tr>
<td>Fujiwara</td>
<td></td>
<td>LMTO</td>
<td>4.50</td>
</tr>
<tr>
<td>Mattheiss</td>
<td></td>
<td>LAPW</td>
<td></td>
</tr>
<tr>
<td>Pickett</td>
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<td>LAPW</td>
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</tbody>
</table>

As has been reported, the conduction bands arise mainly due to the overlap of the Cu-3d and O1-2p wavefunctions. The density of states as well as the partial density of states at the Fermi energy are given in table 2. The deviation in the value of \( N(E_F) \) from other LMTO calculations is due to the following factors: 1. the number of mesh points for which the eigenvalues are calculated 2. the accuracy to which the eigenvalues are calculated and 3. the type of the exchange correlation scheme used in the construction of the potential.

We have used the same lattice parameters and exchange correlation scheme as used by Fujiwara and Hatsugai and it is satisfactory to note that \( N(E_F) \) value is in close agreement with that of Fujiwara and Hatsugai. The present calculation lends support to the recently made observation of Pickett (1989) with regard to the over all agreement between the theoretical and experimental densities of states. The conduction band width and the electronic specific heat coefficient are explicitly given in the present work.

This work was supported by UGC superconductivity project. One of the authors (GS) acknowledges the financial support from the CSIR-SRF grant.

References

Fujiwara T and Hatsugai Y 1987 Jpn. J. Appl. Phys. 26 L716
Oguchi T 1987 Jpn. J. Appl. Phys. 26 L417
Pickett W E 1989 Rev. Mod. Phys. 61 433
Skriver H L The LMTO method (Berlin: Springer Verlag) September 1984
Ta..egahara K, Harima H and Yanase A 1987 Jpn. J. Appl. Phys. 26 L352