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Electronic structure and contact field trend in high-T_c superconductors

E. Pavarini[1], O. Jepsen[2], O. K. Andersen[2]

[1] *INFM- Dipartimento di Fisica "A.Volta", I-27100 Pavia*

[2] *Max-Planck-Institut FKF, Heisenbergstrasse 1, 70569 Stuttgart, Germany*

In cuprate superconductors the contact field (B) at Cu site (CuO_2 plane) is strongly dependent on the material: in La cuprates such as $La_{2-x}Sr_x$ CuO_4 B is $\sim$ 40 kOe/μ_B, while in Tl and Bi cuprates it is systematically larger (e.g. 150 kOe/μ_B in $Tl_2Ba_2CuO_{6+x}$). In order to explain this behavior, we calculate (ab-intio) and analyze the electronic structure of ~ 15 superconducting cuprates.

We show that the band structure can be understood by using a few-orbital chemical model derived from LDA bands. This model includes four orbitals in the CuO_2 plane (Cu $d_{x^2-y^2}$, O_a p_x, O_b p_y, and Cu $4s$) and some orbitals perpendicular to the plane (Cu d_{3z^2-1}, the apical-oxygen (O_c) p_z and farther orbitals from e.g. Hg or La.) We show that the essential material dependent parameter of the model is the energy of the *axial orbital*, an hybrid between Cu $4s$, O_c p_z and the other perpendicular orbitals[1].

We show that the contact field tends to be larger when the energy of the axial orbital is lower, e.g. it is larger in the systems in which the apical oxygen O_c is farther from the CuO_2 plane. This can explain why B is larger in Tl and Bi cuprates than in La cuprates. In addition, we compare the results from two different pictures: Bloch (or delocalized spins) and Wannier (or localized spins) picture and discuss the consequences of the two pictures for the electronic structure and the contact field.

[1] E.Pavarini et al., cond-mat/0012051.