

Relevance of atomic multiplet structure to models of cuprate layers

Mi Jiang, Mona Berciu, and George Sawatzky

Stewart Blusson Quantum Matter Institute, University of British Columbia, Canada

We calculate the spectra of two holes doped in a CuO_2 layer with Cu-d^{10} and O-2p^6 including the full multiplet structure for both atoms. Distinct from previous studies that treated Cu as an impurity within a featureless O-2p band, we dealt with the lattice of Cu and employed the tight binding band structure to describe the O-2p band. We claim that the combination of the full Cu-3d multiplets and realistic O-2p band structure is important to understand the correlated properties of cuprates. We also explored the connection between this model and the conventional three-orbital Emery model in terms of the renormalization of Cu-O hybridization.

[1] H. Eskes, L.H. Tjeng, and G.A. Sawatzky, Phys. Rev. B **41**, 288 (1990).