First-Principles Construction of the Zhang-Rice singlet: Role of the apical oxygen in the mobility of the doped hole.\textsuperscript{1} WEI KU, WEI-GUO YIN, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973 — The Zhang-Rice singlet (ZRS) has been well accepted as the most relevant low-energy states in high $T_c$ cuprates. Based on a novel Wannier state analysis [1] of the LDA+$U$ electronic structure, a realistic ZRS is constructed from properly orthogonalized local Cu $d_{x^2-y^2}$ and symmetric combination of O-$p$ states ($p^{(s)}$), leading to a realistic derivation of low-energy effective $t$-$t'$-$t''$-$J$ Hamiltonian. Interestingly, symmetrized apical oxygen $p_z$ orbital with the Cu $d_{z^2}$ symmetry is found to be close to the ZRS in energy (0.7 eV) and thus significantly facilitates the hopping to the second and third nearest neighbors. [1] W.-G. Yin, D. Volja, and W. Ku, cond-mat/0509075.

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