Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First-Principles Construction of the Zhang-Rice singlet: Role of the apical oxygen in the mobility of the doped hole.[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.

[1]Work supported by DOE-CMSN

Wei K
Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, NY 119

Date submitted: 30 Nov 2005 Electronic form version 1.4