Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Tuning effective interactions in high-T_c cuprates via apical oxygen atoms: New realization from the first-principles Wannier function approach WEIGUO YIN, WEI KU, Brookhaven National Laboratory — Based on a novel first-principles Wannier function approach, the low-energy effective Hamiltonian for high-T_c cuprates is derived. The apical oxygen atoms are found to significantly modify the mobility and distribution of the Zhang-Rice singlets in the CuO_2 plane, by tuning the effective hopping parameters t' and t'', and local chemical potential, $\mu_{\rm eff}$. Most remarkably, $V_{\rm eff}$, an additional effective repulsion (depairing) between neighboring doped holes, is found to be significantly tuned by a "vacuum fluctuation" mechanism inherited from the correlated multiband nature of the cuprates. Our results identify the apical oxygen states as the main material dependence of these systems and provide a microscopic avenue to the understanding of recent spectroscopic imaging STM data [K. McElroy *et al.*, Science **309**, 1048 (2005)].

Weiguo Yin
Brookhaven National Laboratory

Date submitted: 03 Dec 2006 Electronic form version 1.4