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, $\mu_{\text{eff}}$. Most remarkably, $V_{\text{eff}}$, 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)].