Abstract Submitted
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Tuning Hole Mobility, Distribution and Repulsion in High-T_c Cuprates via Apical Atoms[1] WEI KU, CMPMSD, Brookhaven National Lab; Physics Department, State University of New York, Stony Brook, WEI-GUO YIN, CMPMSD, Brookhaven National Lab — Using a newly developed first-principles Wannier-states approach that takes into account large on-site Coulomb repulsion, we derive the low-energy effective one-band interacting Hamiltonians for several prototypical cuprate superconductors. The material dependence is found to originate primarily from the different energy of the apical atom p_z state. Specifically, the general properties of the low-energy hole state, namely the Zhang-Rice singlet, are significantly modified, via additional intra-sublattice hoppings, nearest-neighbor "super-repulsion," and other microscopic many-body processes. Possible implications on modulation of local pairing gaps, charge distribution, hole mobility, electron-phonon interaction, and multilayer effects will be discussed.

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