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Calculated Zhang-Rice Singlet Dispersion in Mott-Insulators XIANGANG WAN, QUAN YIN, SERGEY SAVRASOV, University of California, Davis — Using a combination of local density functional theory and cluster exact diagonalization based dynamical mean field theory (LDA+DMFT), we calculated many body electronic structures of several Mott-insulating oxides including undoped prototype high Tc materials. The dispersions of the lowest occupied electronic states are associated with the Zhang-Rice singlets (ZRS) in cuprates, and with doublets, triplets, quartets and quintets in more general cases. The spectral weight of ZRS band decreases as it approaches the BZ center, as observed by many recent ARPES experiments. Our results are in good agreement with experiments

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