Evolution of Mid-gap States and Residual 3-Dimensionality in Cuprates

S. SAHRAKORPI, Northeastern University, M. LINDROOS, Tampere University of Technology, R. MARKIEWICZ, Northeastern University, A. BANSIL, Northeastern University — We have carried out extensive first principles doping-dependent computations of angle-resolved photoemission (ARPES) intensities in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \) (Bi2212) and \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (LSCO) over a wide range of binding energies.\(^1,2,3\) Intercell hopping and the associated 3-dimensionality, which is usually neglected in discussing cuprate physics, is shown to play a key role in shaping the ARPES spectra. Despite the obvious importance of strong coupling effects (e.g. the presence of a lower Hubbard band coexisting with mid-gap states in the doped insulator), a number of salient features of the experimental ARPES spectra of LSCO are captured to a surprising extent when \( k_z \)-dispersion is properly included in the analysis.


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