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Charge transfer insulators at half-filling in multiband models of cuprates¹ PETER MISTARK, CHRISTOPHER LANE, Northeastern University, HSIN LIN, National University of Singapore, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — Self-consistent mean-field three-band and four-band Hubbard models are used to study the collapse of the Mott gap in doped cuprates. While no set of doping-independent parameters can explain the observed gaps for the entire doping range, the experimental results are consistent with a weakly doping dependent Hubbard U . A key finding is that, when the Cu-O splitting energy Δ is large, the cuprates behave as Mott insulators. However, for small Δ , the cuprates become charge transfer insulators.

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