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Raising Bi-O bands above the Fermi energy level of hole-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and other cuprate superconductors HSIN LIN, S. SAHRAKORPI, R.S. MARKIEWICZ, A. BANSIL, Northeastern University — The Fermi surface (FS) of $Bi_2Sr_2CaCu_2O_8$ (Bi2212) predicted by band theory displays Bi-related pockets around the $(\pi, 0)$ point, which have never been observed experimentally. We show that when the effects of hole doping by substituting Pb for Bi or by adding excess O in Bi2212 are included, the Bi-O bands are lifted above the Fermi energy (E_F) and the resulting first-principles FS is in remarkable accord with measurements. With decreasing hole-doping the Bi-O bands drop below the E_F and the system self-dopes below a critical hole concentration. Computations on other Bi- as well as Tl- and Hg-based compounds indicate that lifting of the cation-derived band with hole doping is a general property of the electronic structures of the cuprates. Work supported by the USDOE.

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