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Different doping from apical and planar oxygen vacancies in $Ba_2CuO_{4-\delta}$ and $La_2CuO_{4-\delta}$ THOMAS JARLBORG, DPMC, 24 Quai E-Ansermet, University of Geneva, CH1211 Geneva 4, BERNARDO BARBIELLINI, ROBERT MARKIEWICZ, ARUN BANSIL, Dep. of Physics, Northeastern University, Boston, Mass 02115, USA — First principles band-structure calculations for large supercells of $Ba_2CuO_{4-\delta}$ and $La_2CuO_{4-\delta}$ with different distributions and concentrations of oxygen vacancies show that the effective doping on copper sites strongly depends on where the vacancy is located. A vacancy within the Cu layer produces a weak electron doping effect while a vacancy located at an apical oxygen site acts as a stronger electron dopant on the copper layers and gradually brings the electronic structure close to that of $La_{2-x}Sr_xCuO_4$. These effects are very robust and only depend marginally on lattice distortions. Our results show that deoxygenation can reduce the effect of traditional La/Sr or La/Nd substitutions. Our study clearly identifies location of the dopant in the crystal structure as an important factor in doping of the cuprate planes.

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