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Interplay of Ca and O doping in $\mathbf{Y_{1-x}Ca_xBa_2Cu_3O_{6+y}}$ studied by first-principles calculations VINCENZO FIORENTINI, ALESSIO FILIPPETTI, DANILO PUGGIONI, CNR-INFM SLACS and University of Cagliari — Experiments reveal an impressive asymmetry in most aspects (involving e.g. magnetic, superconducting, or structural properties) of high-Tc superconductors upon cation or oxygen doping, respectively. A thorough understanding of this asymmetry cannot eschew a rigorous description of the fundamental mechanism ruling electronic and structural properties for each (x,y) doping combination. Here we present results obtained by the pseudo-self-interaction free density functional (pSIC) method, which is capable to describe metal-insulating transitions in several cuprate materials. We describe in detail the chemistry of the distinct insulating-metal transitions occurring in the CuO chains and in the CuO_2 planes in underdoped $YBa_2Cu_3O_{6+y}$for y=[0,0.5]. We then show that interactions with chains crucially affect the ability of Ca doping to inject holes in CuO_2 planes. The dramatic effects of this double-doping interplay on the magnetic and superconducting properties of underdoped $Y_{1-x}Ca_xBa_2Cu_3O_{6+y}$ cannot be understood by the disentangled action of the individual doping sources.

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