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Holes localization and Fermi Surface morphology of $Y_{1-x}Ca_xBaCu_3O_6$ by First-Principles GIORGIA LOPEZ, ALESSIO FILIPPETTI, VINCENZO FIORENTINI, University of Cagliari, Italy — The basic chemistry of underdoped $Y_{1-x}Ca_xBaCu_3O_6$ (and of high-T_c superconductors) is permeated by unexplained features. One, in particular, concerns the nature of the non- superconducting phase and its Fermi Surface (FS) whose character is not univocally described by angle-resolved photoemission and Hall measurements, which detect disconnected arcs and pockets, respectively. But what is really missing for a sound interpretation of these data is a robust link between the observed FS and the corresponding electronic structure. As the description of the underdoped regime is hardly accessible through standard First-Principles calculations (FPC), here we use the innovative pseudo-self-interaction corrected local spin density (PSIC) approach to trace an accurate overview of underdoped $Y_{1-x}Ca_xBaCu_3O_6$, with special emphasis on the FS morphology. In particular, the PSIC can predict the formation of Zhang-Rice singlets (ZRS), and we show that electronic states characterized by a mixture of ZRS and antiferromagnetic CuO_2 units present, in fact, a variegated series of differently-shaped, disconnected FS that may reconcile the experimental data with a sound interpretation of the underdoped $Y_{1-x}Ca_xBaCu_3O_6$ properties.

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