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Band-theory description of hole localization and singlet polarons in doped cuprates ALESSIO FILIPPETTI, DANILO PUGGIONI, VINCENZO FIORENTINI, CNR-INFM SLACS and University of Cagliari, CNR-INFM SLACS TEAM — We use an advanced ab-initio band theory (the pseudo-self interaction corrected local density approach, pSIC) to describe spin-compensated polarons (e.g. Zhang-Rice singlets (ZRS)) typical of low-dimensional doped cuprates. Despite their many-body nature, ZRS can be transparently interpreted via (and, in fact, constructed from) single-particle states, provided that band theory describes accurately enough their localization in the limit of vanishing band dispersion. We provide examples of polarons in real materials, specifically chain-like $\text{Ca}_{2+x}\text{Y}_{2-x}\text{Cu}_5\text{O}_{10}$ and the high- T_c superconductor (HTSC) $\text{Y}_{1-x}\text{Ca}_x\text{Ba}_2\text{Cu}_3\text{O}_{6+y}$. The former is the ideal prototype of dopable one-dimensional cuprate with zig-zag Cu-O interactions. Studying the electronic and magnetic properties over the full range of possible doping, we identify several different polaron-dominated ground states and the attendant phase transitions. Furthermore, ZRS are key to the behavior of doped CuO_2 units in HTSC. We show how their occurrence can dramatically affect the electronic properties (e.g. the Fermi surface) in underdoped $\text{Y}_{1-x}\text{Ca}_x\text{Ba}_2\text{Cu}_3\text{O}_{6+y}$.

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