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Metal-insulating transition and Zhang-Rice singlets in one-dimensional cuprates: the case of $\mathbf{Ca_{2+x}Y_{2-x}Cu_5O_{10}}$ ALESSIO FILIPPETTI, VINCENZO FIORENTINI, University of Cagliari, Italy — Chain-like $Ca_{2+x}Y_{2-x}Cu_5O_{10}$ is the ideal prototype of dopable one- dimensional cuprate with zig-zag Cu-O interactions. The observed abundance of Zhang-Rice singlets in the electronic ground state of the system induces peculiar phase transitions in magnetic and conducting properties upon doping. With the use of unconventional first-principles calculations suited for to the study of strong-correlated materials, we describe the change of electronic and magnetic properties as doping is varied from x=0 to full-doped concentration (i.e. one hole each CuO_2 unit). Zhang-Rice singlets are key ingredients to understand the behavior of doped CuO2 units and the rise of high-Tc superconductivity in cuprates. We can visualize ZR singlets in space and energy at varying doping concentration, and their influence on magnetic and dielectric properties. ZR singlets are associated to holes localization on the oxygens, appear for holes concentration above 0.25 per CuO_2 and persist up to maximum doping (i.e. one hole per CuO_2) that is well above the threshold of the metallic regime. Our findings are indicative of the general behavior of low-dimensional doped cuprates and give evidence that first-principles band-energy approaches can be valuably employed to the study of doped cuprates.

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