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Metal to insulator transition and ground state electronic structure of $\mathbf{La_{2-x}Sr_xCuO_4}$[1] T.C. SCHULTHESS, Oak Ridge National Laboratory, W.M. TEMMERMAN, Z. SZOTEK, Daresbury Lab., P.R.C. KENT, U. of Tennessee — We use the self-interaction corrected local spin-density (SIC-LSD) method to study the ground state electronic structure of $La_{2-x}Sr_xCuO_4$ as a function of Sr doping x. SIC-LSD is a parameter free method based on Density Functional Theory that has proven reliable for the study of strongly correlated electron systems. Sr is introduced via the virtual crystal approximation by linearly mixing the La and Sr potentials. In our calculations, we find that the nature of Cu-$d_{x^2-y^2}$ orbital changes character with varying Sr concentration. In the under-doped regime, one of the Cu-$d_{x^2-y^2}$ orbitals per atom is fully occupied and localized on the Cu site, leading to the formation of magnetic moments on Cu aligned antiferromagnetically in the CuO2 plane. Sr doping introduces holes mainly into the O-p bands and the system is a doped charge transfer insulator. In the over-doped regime, the Cu-$d_{x^2-y^2}$ orbitals are band-like and not spin-split. The moments on the Cu atoms vanish and the system is a nonmagnetic metal. In the orthorhombic structure, the transition from localized to band-like Cu-$d_{x^2-y^2}$ states occurs at about18% Sr doping, i.e. within the region of optimal doping for superconductivity. We find a similar behavior if the calculations are performed with the idealized tetragonal structure.

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