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Spin-state controlled electronic and magnetic structures of $Sr_{2-x}La_xCoO_4$ HUA WU, Fudan University, Shanghai, China — $Sr_{2-x}La_xCoO_4$ is an interesting group of materials, and they display abundant electronic and magnetic properties. In this work, we studied those properties, using electron-correlation corrected density functional calculations. We find that besides a charge-state variation induced by La doping, a multiple spin-state transition takes place and determines (1) a metal-insulator transition and a ferromagnetic insulating phase for x=0.5 [1], (2) a paramagnetic Mott insulating phase with a mixed high-spin and low-spin state for x=1, instead of a ferromagnetic half-metallic solution with a homogeneous intermediate-spin state [2], and (3) a charge-ordered highly insulating phase with an active spin-blockade mechanism for x=1.5 [3]. [1] H. Wu, Phys. Rev. B 86, 075120 (2012). [2] H. Wu, Phys. Rev. B 81, 115127 (2010). [3] H. Wu and T. Burnus, Phys. Rev. B 80, 081105(R) (2009).

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