Structural, magnetic and electronic properties of strained $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) crystals studied by ab-initio calculations.

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$La_{0.67}Sr_{0.33}MnO_3$ (LSMO) bulk under strong hydrostatic pressure and uniaxial strain has been studied with three DFT based approaches, i.e. the GGA, the GGA+U, and the PSIC (pseudo self interaction correction). As for the structural properties of the ferromagnetic (FM) phase our calculations show that under hydrostatic pressure the octahedra rotations are reduced and no Jhan-Teller distortions are present. The antiferromagnetic (AF) phases are always disfavoured at all the simulated pressure although they are strongly strengthened by the compression. The AF (metallic) phases competition vs. the FM (half metallic) phase was found to be strongly helped by the JT distortions which necessarily appear in LSMO crystals when a planar strain (corresponding to the experimental growth on $LaAlO_3$ and $YALO_3$ substrates) was applied in our simulations: the AF-a order becomes favoured for a system under a planar a vertical compression , while a vertical tension stabilizes the AF-c phase. Thus, our conclusion is that under compression double exchange (DE) weakens (not strengthens, as usually believed) along the applied strain direction as a consequence of carriers depletion at the Fermi energy and of the consequent p-d hybridisation decrease. This work shows that First-Principles calculations represent a capable tool complement to the experiments fundamental in order to design manganese-based devices with improved functionalities.

9.7 cm

13.4 cm

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