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Electronic structure of the (001) surface of half-metallic manganites MIGUEL PRUNEDA, UC Berkeley, VALERIA FERRARI, CNEA Argentina, PETER B LITTLEWOOD, EMILIO ARTACHO, University of Cambridge — A good understanding of the physical properties of surfaces and interfaces of in colossal magneto-resistant hole-doped manganese oxides is highly desirable for future applications of these promising materials in magnetoresistive devices for spintronics. We present results for a fully relaxed (001) surface in the optimally doped half-metallic manganites $La_{0.7}Sr_{0.3}MnO_3$ in its distorted orthorhombic phase, based on density functional calculations with explicit doping. The crystal termination gives rise to a splitting in the degenerate t_{2g} and e_g levels, and a surface state with $d_{z^2} + d_{xy}$ character develops. The calculations for the relaxed structure show that the tilting of MnO_6 octahedra is reduced near the surface, and there is a layer buckling, with a Mn off-centering in the top octahedral layer similar to what observed for Ti in bulk $BaTiO_3$, which decreases rapidly inside the material. As a result of this distortions, the surface state shifts to lower energies, although it is still very localized in the first layer. The Mn off-centering favours the occupation of the conduction d_{z^2} states, which become more localized and affects the magnetic properties at the surface.

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