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First-principles study of the electronic and magnetic properties of $\mathbf{La_{1-x}Sr_xMnO_3}$ and $\mathbf{La_{1-x}Ca_xMnO_3}$[1] M.-H. TSAI, Y.-H. TANG, H. CHOU, National Sun Yat-Sen University — Using spin-polarized first-principles calculations, we find that the observed insulator behavior of $LaMnO_3$ is due to the existence of a trough in the total density of states, D(E), just above the Fermi level, E_F. D(E) in this trough, though not zero, is very small, so that $LaMnO_3$ has a high resistivity at low temperature. The trough is similar to an energy gap, so that the resistivity decreased with temperature. The observed optical energy gap is due to that the states immediately above E_F have the same orbital symmetry as those immediately below E_F. $LaMnO_3$ has a deficiency of majority-spin e_g states immediately above E_F, so that the O mediated super-exchange coupling dominates and the material is antiferromagnetic. The calculated spin-polarized partial densities of states of $La_{1-x}Sr_xMnO_3$ and $La_{1-x}Ca_xMnO_3$ show that Sr and Ca induce delocalization of majority-spin e_g states, which render these materials semimetallic. The empty majority-spin e_g states immediately above E_F enhance delocalized-state mediated Mn-Mn spin couplings, so that these materials are ferromagnetic. Another effect of Sr and Ca doping is the lowering of the minority-spin e_g band down to E_F, which may explain colossal magnetoresistance.

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