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Search for Half-Metallic Antiferromagnetism in Double Perovskites V. PARDO, Univeristy of California Davis, W. E. PICKETT, University of California Davis — The wide class of double perovskite oxides was proposed earlier (PRB 57, 10613 [1998]) as promising for producing a half-metallic antiferromagnet [HMAFM] (more correctly, a spin-compensated half metal). Here we present examples of the affects of structural distortions on the electronic and magnetic properties in selected members. For La_2CrNiO_6 the idealized cubic perovskite structure had led to a spin-antiparallel state with net moment of 0.6 μ_B, but a ferromagnetic half-metallic state (4 μ_B) was 150 meV per metal atom lower in energy (within local density approximation). Starting with experimental information on $LaCrO_3$ and $LaNiO_3$ and their alloys, we have relaxed the volume and the (seven) internal coordinates within the orthorhombic Pnma space group. The charge states can be characterized by Cr^{4+} and Ni^{2+}. The ferromagnetic state is lower by 50 meV within the generalized gradient approximation. Using LDA+U (U=3 eV on each transition metal ion) opens a gap of 0.6 eV (FM insulator) and is favored by 120 meV over the antialigned state. Although no HMAFM state is obtained, these results show that structural relaxation must be taken into account, and that in some cases (as here) it may make the antialigned state more favorable.

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