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Electronic structures of non-half-metallic antiferromagnetic double perovskites ALaVMoO$_6$ (A = Ca, Sr, and Ba)[1] I.G. KIM, A.J. FREEMAN, Northwestern University, M.S. PARK, B.I. MIN, POSTECH, Pohang, Korea — Recently, double perovskites ALaVMoO$_6$ (A = Ca and Sr) of the $Fm\bar{3}m$ space group were proposed experimentally to be half-metallic antiferromagnets.[2] The electronic structures and magnetism of the double perovskites ALaVMoO$_6$ (A = Ca, Sr, and Ba) were determined within the generalized gradient approximation to density functional theory using the all-electron full-potential linearized augmented plane wave (FLAPW) method.[3] The A = Ca case shows *metallic* ferrimagnetism as the most stable phase, with magnetic moments of 1.15 μ_B for V and -0.53 μ_B for Mo, whereas the Sr and Ba cases are calculated to be almost non-magnetic metals. Comparing the calculated density of states, we find that the heavier A implies stronger hybridization between the divalent atom *sp* states and the transition metal atom *d* states. The stronger *sp*-*d* hybridization is considered to be responsible for the suppression of magnetism for the Sr and Ba cases. These results, at least for the $Fm\bar{3}m$ space group, are in contrast with the recent experimental result proposing half-metallic antiferromagnetism for A = Ca and Sr.

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[2]Uehara, Yamada, and Kimishima, Solid St. Commun. **129**, 385 (2004).
[3]Wimmer, Krakauer, Weinert, and Freeman, PRB **24**, 864 (1981).

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