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First-principles exploration of multiferroic oxides with double-perovskite structure TAMIO OGUCHI, TATSUYA SHISHIDOU, YOSHITAKA URATANI, ADSM, Hiroshima University — Multiferroics have attracted much attention recently because of their novel properties. There are a few known as ferromagnetic and ferroelectric materials, particularly with perovskite-type crystal structure. Ferroelectrics should be insulating and likely ionic. Furthermore, it is widely recognized that covalent bonds between the cation and anion orbitals are crucial to realize atomic displacements to a noncentrosymmetric structure. As for magnetism, most of magnetic perovskite oxides usually have an antiferromagnetic order (mostly frustrating) due to a superexchange coupling. According to the Kanamori-Goodenough rule for the superexchange coupling, certain combinations of the transition-metals ions (d^3-d^5 and d^3-d^8 configurations) may possibly give a ferromagnetic coupling by the 180° superexchange mechanism. In this study, we explore possible co-existence of spontaneous electric polarization and ferromagnetic ordering from first principles, by focusing bismuth double-perovskite oxides $Bi_2BB'O_6$ ($B, B' = 3d$ ions) as target materials. Ferromagnetic and ferrimagnetic solutions are obtained for cubic Bi_2MnNiO_6, Bi_2CrFeO_6 and Bi_2CrCuO_6 with nearly gapped electronic structure. Quite recently, Bi_2MnNiO_6 has been successfully synthesized by a high-pressure technique and revealed multiferroic properties. Possible multiferroic properties of Bi_2MnNiO_6 with the observed monoclinic structure are investigated in detail.

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