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First-Principle Calculations of Half-Metallic Double Perovskite $La_2BB'O_6$ ($B,B' = 3d$ transition metal)

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Abstract. In this paper, we present calculations based on density functional theory using generalized gradient approximation (GGA) in double perovskite structure $La_2BB'O_6$ ($B,B' = 3d$ transition metal) out of 45 (C_2^{10}) combinational possibilities. Considering 4 types of magnetic states, namely, ferromagnetic (FM), ferrimagnetic (FiM), antiferromagnetics (AF), and nonmagnetic (NM) with full structure optimization, 13 possible surviving, stable FM/FiM-HM materials containing 6 FM-HM materials (La_2ScNiO_6, La_2CrCoO_6, La_2CrNiO_6, La_2VScO_6, La_2VZnO_6, and La_2VNiO_6) and 7 FiM-HM materials (La_2VFeO_6, La_2ZnCoO_6, La_2TiCoO_6, La_2CrZnO_6, La_2CrMnO_6, La_2ScFeO_6, and La_2TiMnO_6) are found. Considering the correlation effect (GGA+U), there are 6 possible half-metallic stable, surviving (HM) materials containing 3 FM-HM materials (La_2ScNiO_6, La_2CrCoO_6, and La_2CrNiO_6) and 3 FiM-HM materials (La_2VFeO_6, La_2ZnCoO_6, and La_2TiCoO_6).

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Key words: Half-metallic materials, double perovskites structure, first-principle density functional theory.

1 Introduction

In ordered double perovskites denoted as $A_2BB'O_6$ (A=alkaline-earth or rare-earth ion, B and B'=transition metal ion), the differences in the valance and size between the B

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and B' cations are crucial for controlling the physical properties [1, 2]. Among them, Sr_2FeMoO_6 [3] has been discovered to possess colossal magneto resistance (CMR) at room temperature. The high transition temperature T_c and low field magnetoresistance indicate half-metallic (HM) behavior in this compound. In HM materials, there is a well-defined gap in the majority channel and a metallic behavior in the minor spin channel. Thus, HM materials have three properties: (1) quantization of the magnetic moment; (2) 100% spin polarization at the Fermi level; (3) zero spin susceptibility. Due to their single-spin charge carriers, HM materials can be used in creating computer memories, magnetic recordings, and so on.

This work searches for new HM materials in all the 45 (C_2^{10}) double pervoskite structure of $La_2 3d 3d' O_6$ series, where $3d3d'$ pairs are combinations of all $3d$ transition elements. The research is based on the first-principle generalized gradient approximation (GGA) calculations, with the consideration of four types of magnetic states, namely, ferromagnetic (FM), ferrimagnetic (FiM), antiferromagnetics (AF), and nonmagnetic (NM), in ideal cubic structure ($Fm\bar{3}m$, No. 225). Up to 22 possible compounds were obtained from the first round of filtering calculation. After the structural optimization process and considering the energy difference between the 4 magnetic states, 13 possible FM/FiM-HM materials proved to be stable containing 6 FM-HM materials (La_2ScNiO_6, La_2CrCoO_6, La_2CrNiO_6,La_2VScO_6, La_2VZnO_6, and La_2VNiO_6) [27] and 7 FiM-HM materials (La_2VFeO_6, La_2ZnCoO_6, La_2TiCoO_6, La_2CrZnO_6, La_2CrMnO_6, La_2ScFeO_6, and La_2TiMnO_6). In transition metal oxides, the strong electron correlation systems need better description rather than GGA calculations. However, GGA calculations can be corrected using a strong-correlation correction called GGA(LDA)+U method. In the GGA+U process, U and J stand for Coulomb and exchange parameters, respectively, and the effective parameter $U_{eff} = U - J$ is adopted. In this paper, we used U instead of U_{eff} for simplicity. Our result matched that of a previous study, which indicates that La_2NiFeO_6 [4] and La_2ZnRuO_6 [5] are HM materials upon which La_2NiFeO_6 needs to base the GGA+U calculations on; La_2VMnO_6 [6] and La_2VCuO_6 [7, 8] are half-metallic antiferromagnetics (HM-AFM) where La_2VMnO_6 needs to go through for full structural optimization calculation; and La_2NiMnO_6 [9–11] is a ferromagnetic insulator (FM-Is) material. Based on our result, La_2ScNiO_6, La_2CrCoO_6, and La_2CrNiO_6 are half-metallic ferromagnetic (FM-HM) compounds and La_2VFeO_6, La_2ZnCoO_6, and La_2TiCoO_6 are half-metallic ferrimagnetic (FiM-HM) materials.

2 Computational method

The theoretical research was based on density functional theory (DFT) [12], and using GGA [13] to approach the exchange-correlation potential. The structural optimization (i.e., relaxation for both lattice constants and atomic positions) were carried out using the full-potential projector augmented wave (PAW) [14] method and the conjugate-gradient (CG) method as implemented in the VASP code [15, 16], which is fast and efficient. To