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Magnetic and thermoelectric properties of ordered double perovskite Ba_2FeMoO_6

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Abstract

The structural, magnetic and electronic properties of ordered double perovskite Ba_2FeMoO_6 has been calculated with the full potential linearized augmented plane wave (FPLAPW) method. Spin polarization calculations for this compound show half metallic ground state with the ferromagnetic coupling of Fe and Mo spins; the magnetic moment amounts to μ_{Fe} = 3.631 μ_B, whereas no magnetic moment was found on the Mo site within the experimental error, which is consistent with experimental observation. Based on the electronic results, the temperature dependence of the thermoelectric properties of Ba_2FeMoO_6 was investigated in temperature range from 200 to 1200 K. The Seebeck coefficient became negative indicating n-type semiconducting behavior of Ba_2FeMoO_6 in the whole temperature range. Our results indicate that the highest dimensionless figure of merit ZT≈1 was obtained at 200K.

Keywords: Half-metallic, ferromagnetic, double perovskite, FP-LAPW method.

Introduction

Bulk thermoelectric materials have involved significant interest in the field of energy conversion technology due to their potential in the conversion of waste heat to electrical power [1-2]. They are required to have a large value of the dimensionless figure of merit $ZT = S^2T/\rho\kappa$, where S, ρ, κ and T are the Seebeck coefficient, the resistivity, the thermal conductivity and the absolute temperature, respectively [3]. Accordingly, they have to exhibit all together low resistivity, low thermal conductivity and large Seebeck coefficient. Such materials are, however, rarely found because the three parameters are functions of carrier concentration in conventional semiconductors and they cannot be easily controlled independently. The family of double perovskite compounds with general formula ABB'O_6, has provided materials of high technological applications, namely spintronic materials (Sr_2FeMoO_6), multiferroic material (Bi_2NiMnO_6), magneto-dielectric materials (La_2NiMnO_6, La_2CoMnO_6), and magneto-optic materials (Sr_2CrWO_6, Sr_2CrReO_6, Sr_2CrOsO_6) [4-7]. In contrast to the compounds that constitute the family of double perovskites broadly studied experimentally and by means of ab initio calculations, Ba_2FeMoO_6 is much less investigated due to its lower Tc of 308 K [8]. This material exhibiting both ferromagnetic and half-metal character possess an unusual electronic structure. An additional peculiarity of its electronic properties is that all the conduction electrons are completely spin-polarized in the vicinity of the Fermi level, which show promise for improving the figure of merit ZT by enhancing the electrical conductivity and the Seebeck coefficient. In the present study, we establish the basic structural, magnetic and electronic properties of the ordered double perovskite Ba_2FeMoO_6 using the FP-LAPW method. In addition, we investigate the thermoelectric properties of this compound using Boltzmann transport theory.

Computational details