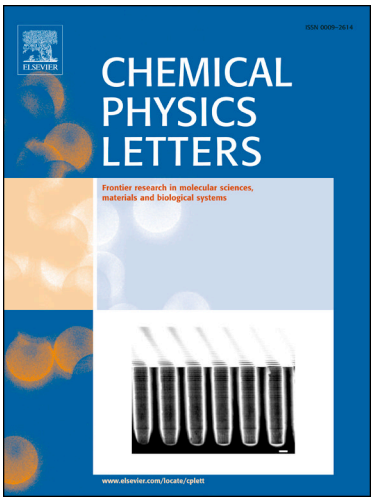

Research paper

Magnetic and electronic properties of double perovskite Lu_2MnCoO_6:*Ab-initio* calculations and Monte Carlo simulation

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Magnetic and electronic properties of double perovskite Lu_2MnCoO_6: *Ab-initio* calculations and Monte Carlo simulation

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Abstract:

The magnetic and electronic properties of the double perovskite Lu_2MnCoO_6 are studied by combining the *ab-initio* calculations and Monte Carlo simulation (MCs) based on the Ising model. This compound is constituted of two magnetic cubic sublattices: one occupied by Mn^{4+} with spin (s=3/2) and other occupied by Co^{2+} with spin (σ =3/2). By using *ab-initio* calculations we compute the exchange coupling between Mn-Co sublattices. We also investigate the phase transitions and the magnetic stability of this compound. The Curie temperature is determined as well as the critical exponents. We show that the Lu_2MnCoO_6 compound belongs to the 3D-Ising universality class.

Keywords: Magnetic properties; *Ab-initio*; Lu_2MnCoO_6; Monte Carlo Simulation; critical exponents.

1. Introduction

The perovskite compounds have been described in many previous publications [1, 2]. Recently, these compounds received considerable attention and interest intensively with experimental and theoretical studies because of their potential applications. Among these last, there are the magnetic memories [3, 4], tunnel junction [5] spintronics field [6, 7] sensors, microwave and high-power applications [8-10]. The reference of this family has a general formula $A_2BB'O_6$ with A is an alkaline earth cation, the B and B' must be transition metal and O is oxygen [11, 12]. A recent study showed that the Lu_2MnCoO_6 is a new member of the multiferroic oxides. It is subject of interesting studies because of its long-range electric and magnetic order. Yáñez-Vilar et al.[13] indicate that below 35 K, Lu_2MnCoO_6 possesses a strong electric polarization to a net magnetization, despite the antiferromagnetic ordering of the S = 3/2 Mn^{4+} and Co^{2+} spins in an ↑↑↓↓ configuration along the c-axis. This behavior is similar to those found by Choi et al. in Ca_3MnCoO_6 [14, 15] where ↑↑↓↓ magnetic order is observed along the chains Co-Mn-Co-Mn ions, with the difference that the Co^{2+} ion is in the σ = 1/2 state rather than the σ = 3/2 state. In general, Co^{2+} exhibits two different electronic configurations depending on the occupation of t_{2g} and e_g orbitals. The configurations for high spin (HS) and low spin (LS) are $t^7_{2g}\, e^0_g$ (σ =3/2) and $t^5_{2g}\, e^2_g$ (σ =1/2) respectively, while for Mn^{4+} is $t^3_{2g}\, e^0_g$ (S=3/2).