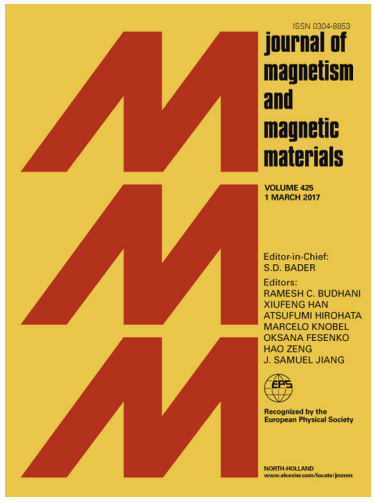

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The Itinerant magnetism in a 3d-4d double perovskite Sr_2CrMoO_6

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Abstract

In this work, we use the exact diagonalization and Monte Carlo calculations to study magnetic behaviors of the 3d-4d double perovskite Sr_2CrMoO_6. The model is described by a quantum Hamiltonian induced by the hybridization mechanism in Sr_2CrMoO_6 via the double exchange, considering the transition metal Mo^{5+} (σ=1/2, $4d^1$) cation totally non-magnetic and classical core spins S=3/2 located at sites of Cr^{3+} (S=3/2, $3d^3$) cations. We have defined a Hamiltonian matrix and determined eigen-energies which are functions of core spins interactions. At ground state, we have found that the ferromagnetic phase of core spins stabilizes the system for the electronic density *n=0.25*. To study magnetic properties at finite temperature, we have defined an effective magnetic Hamiltonian for spins, approving the Monte Carlo simulations for systems of high sizes. Thus, the exchange coupling effect, the magnetization and the magnetic susceptibility are investigated for different sizes, and the critical temperature is determined.

Keywords: Exact diagonalization, Monte Carlo calculations, hybridization mechanism, magnetic properties, effective magnetic Hamiltonian, critical temperature.

I. Introduction

Half metals are materials with metallic character for one spin direction and insulating for the other [1-3]. This materials type is a precious resource for spintronics where, due to high effects of giant magnetoresistance and tunnel magnetoresistance at room temperature [4, 5], they are used for the conception of various electronic devices such as magnetoresistive reading head and magnetic random access memory.