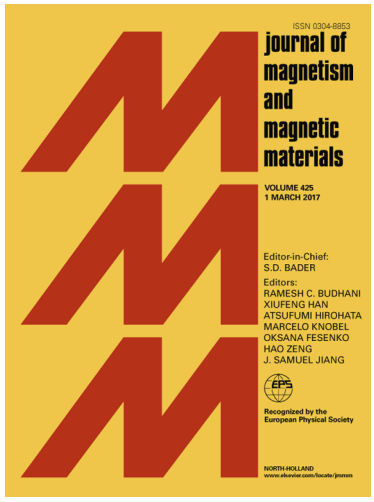

Electronic and magnetic properties of magnetoelectric compound $Ca_2CoSi_2O_7$: an *ab initio* study

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Electronic and magnetic properties of magnetoelectric compound $Ca_2CoSi_2O_7$: an *ab initio* study

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Abstract

The detailed first principle density functional theory calculations are carried out to investigate the electronic and magnetic properties of magnetoelectric compound $Ca_2CoSi_2O_7$. The magnetic properties of this system are analyzed by calculating various hopping integrals as well as exchange interactions and deriving the relevant spin Hamiltonian. The dominant exchange path is visualized with Wannier functions plotting. Only intra planer nearest neighbor exchange interaction is strong in this system. The magnetocrystalline anisotropy is calculated for this system, and the results of the calculation reveal that the spin quantization axis lies in the *ab* plane.

Keywords: Antiferromagnetism, low dimensional spin system, exchange interactions, spinorbit coupling, density functional theory, Wannier function

1. Introduction

The magnetoelectric materials are interesting field of study to both experimentally and theoretically.[1, 2, 3, 4, 5] Due to the coupling of magnetic and electric order parameters, these materials have potential applications in information-storage devices, transducers, sensors, etc. In these materials, electric polarization is often realized by application of magnetic field. The melilite-type compounds with general formula $A_2MM'_2O_7$ have attracted a great deal of

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