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Magnetic properties of the double perovskite Ba_2NiUO_6

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HIGHLIGHTS

- The magnetic properties of the double perovskite Ba_2NiUO_6 are studied.
- The electronic structure is determined.
- The *ab-initio* calculations are performed to determine the density of states.
- The mean field approximation is applied to study the phase diagrams of the double perovskite.
- The Monte Carlo simulations are analyzed and compared with the mean field study.

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ABSTRACT

In this work, we studied the magnetic properties of the double perovskite Ba_2NiUO_6 using the *ab-initio* method, Monte Carlo simulations (MCS), and mean field approximation (MFA). The first method is indispensable for studying and determining the electronic density of states in the framework of the generalized gradient approximation (GGA). The full-potential linearized augmented plane wave (FP-LAPW) method is used in the WIEN2k packages. A theoretical study with mean field approximation and MCS within the Ising model is used to further understand the magnetic properties of this compound. The phase diagrams, the magnetizations, the hysteresis cycles, the specific heat, and the magnetic susceptibilities of this compound have also been studied. The results obtained by these methods are in good agreement with those found in the literature.

1. Introduction

Emerging information technologies and communications require more means of storage and the most advanced processing, especially in the digital form. The development of these resources is under way with both the use of materials with original features and the advent of a new science called spin electronics or spintronics [1]. This new science, the basis of which is materials with high spin polarization, directing research into electron spin, has revolutionized this field.

The materials required in this field include half-metals that are magnetic and with their conduction band totally polarized by spin below their Curie temperature. These semi-metals are singled out from the family of crystalline oxides named the double perovskites with the formula $ABB'O_6$, where conventionally "A" signifies a large electropositive cation, "B" and "B′" represent small transition metals, and "O" is an oxide anion. These materials have been of particular interest in scientific research owing to the following characteristics: magnetoresistance [2], half-metallicity [3], magneto-dielectricity [4], and high magnetic ordering temperatures [5].

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Table 1
The magnetic moment values of all the atomic sites and the total magnetic moment.

Atoms	Magnetic values (μ_B)
Ba	0.0021
Ni	1.5074
U	0.1738
O	0.0534
Total magnetic moment via GGA	1.9975
Experimental value of the total magnetic moment	2.1

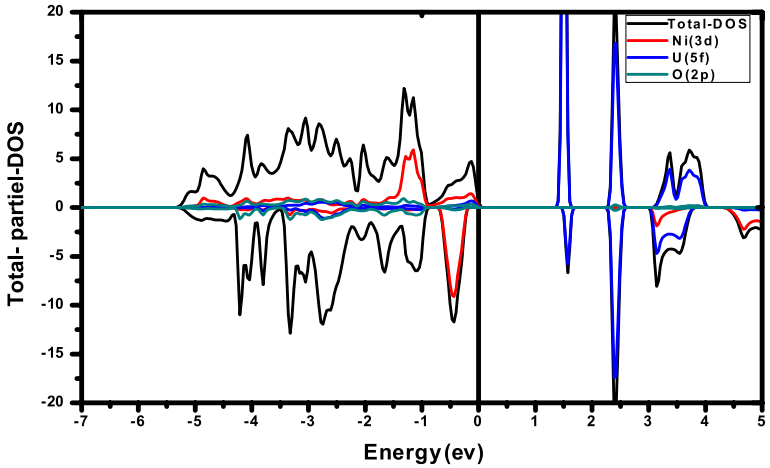

Fig. 1. Total and partial electronic density of states of Ba_2NiUO_6.

The structural data of the compound Ba_2NiUO_6 obtained from the power X-ray patterns have been reported in Refs. [6–10]. The crystal structure of the compound Ba_2NiUO_6 is an undistorted cubic perovskite composite with the space group of $Fm\bar{3}m$. The parameters of this compound are $a = b = c = 8.336$ Å, as established in Ref. [10]. Detailed magnetic susceptibility and specific heat measurements show that the double perovskite Ba_2NiUO_6 orders ferromagnetically at 25 K. This finding was reached by a host of researchers [8,9]. The magnetic properties of this compound are produced by Ni^{2+} ($3S^2 3d^6$, $S = 2$) ions. The U^{6+} ($5f^0\ 6d^0$, $S = 0$) ion is diamagnetic. The experimental moment for the compound Ba_2NiUO_6 is $2.1\mu_B$ as reported in Ref. [9].

The aim of this paper is to study the magnetic properties of the double perovskite Ba_2NiUO_6 using the following simulation methods: *ab-initio*, Monte Carlo, and mean field approximation. These methods are particularly chosen with the aim of studying the magnetic properties of this compound further. Bearing this in mind, we shall determine the density of state, the phase diagrams, the hysteresis loops, the magnetic susceptibilities, as well as the specific heat.

2. *Ab initio* calculation: the study of the electronic density of state

The total and partial electronic densities of Ba_2NiUO_6 compound have been determined by performing calculations within the generalized gradient approximation (GGA) [11] using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [12]. In this manner, as Fig. 1 shows, the calculation of the total and partial electronic density of states (T-PDOS) of Ba_2NiUO_6 generates the following interesting results:

- The valence band consists essentially of the 3d orbital of nickel (Ni) and 2p orbital of oxygen (O), whereas the conduction band is made up of the 5f orbital of uranium (U) and 3d orbital of nickel (Ni).
- The nonsymmetry of the spin-up and spin-down states clearly indicates that the structure has a magnetic character. In other words, the difference between these densities of states, up and down, is not null.
- The compound Ba_2NiUO_6 does not qualify as a half-metal, as no peak is observed at the Fermi level. Hence, it is a magnetic semiconductor.
- Finally, the hybridization is observed between the oxygen layer p and the nickel layer d. Therefore, one can conclude that the exchange coupling p–d is responsible for the magnetism observed in this compound.

Numerically speaking, as Table 1 demonstrates, one can deduce that a large part of the magnetic moment is concentrated in the nickel atom. In the meantime, the remaining part, which is nearly negligible or null, is located in the oxygen, uranium, and barium atoms. In addition, the total magnetic moment value attained by GGA is very close to the experimental result.