Ab-Initio Study of the Ferromagnetic Half-Metallic Perovskite $KMgO_3$

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ABSTRACT

In this work, we investigated the structural, electronic, magnetic and elastic properties of Pérovskite $KMgO_3$, using the Linearized Augmented Plane Wave Method with Total Potential (FP-LAPW) as part of the density functional theory implemented in Wien2k code.

INTRODUCTION

The recent years has seen a lot of research on Pérovskites for potential applications in electronics, photovoltaics, renewable energy and innumerable other industries[1]. The optimized structural parameter of $KMgO_3$ at equilibrium obtained is in good agreement with the results found by other authors; The results show that these compound is stable in the ferromagnetic phase and he has character half-metallic**.**

THEORETICAL STUDY

To study the properties of $KMgO_3$ which is interest in spintronic applications, we performed quantum simulation of first principles "ab-initio" using the formalism of the theory of the functional density[2] to determine with precision a large range of properties of matter. Our DFT calculations are based on full potential linearized augmented plane wave (FP-LAPW[3]). The exchange and correlation potential is treated with the GGA-PBE approximations.

RESULTS AND DISCUSSION

The $KMgO_3$ Pérovskite in the cubic form with space group is Pm-3m (221) contains one formula unit and the K, Mg and O atoms are positioned at 1a (0, 0,0), 1b (½, ½,½) and 3c (0,½, ½) sites of Wyckoff coordinates, respectively. The equilibrium lattice parameter for this compound was obtained from the energy optimization calculations as a function of volume, to determine the structural properties such as lattice parameter a, the modulus of compressibility B and its derivative B' (shown in Table 1)

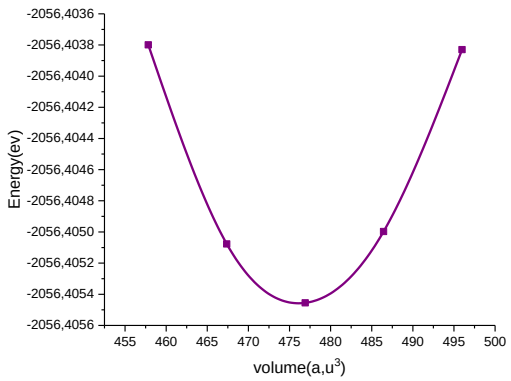

Fig1: Volume optimization of $KMgO_3$

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To investigate the elastic properties, we use IRelast package integrated in the WIEN2k. The study of the elastic properties informs us on the behavior of this compound with regard to the ductility, brittleness and application of the external forces. For compounds that have a cubic structure the elastic constants cij are reduced to only three (c_{11}; c_{12}; c_{44}).

Table1: Calculated values of the lattice parameter a_0, bulk modulus B, its pressure derivation B' and elastic constants C_{11}, C_{12}, and C_{44}

Parameters	Our calc	Other calc
a_0 (Å)	4.1325	4.1344
B(GPa)	63.0911	61.7614
B'(GPa)	4.7480	4.3491
C_{11}(GPa)	130.0052	121.5406
C_{12}(GPa)	32.7361	32.5717
C_{44}(GPa)	14.3281	9.0363

For electronic properties, it is clear in fig 2 that for spin-down states, the compound exhibits a metallic nature but, for the spin-up, the compound shows an insulating nature with half-metallic gaps of 7.285ev.

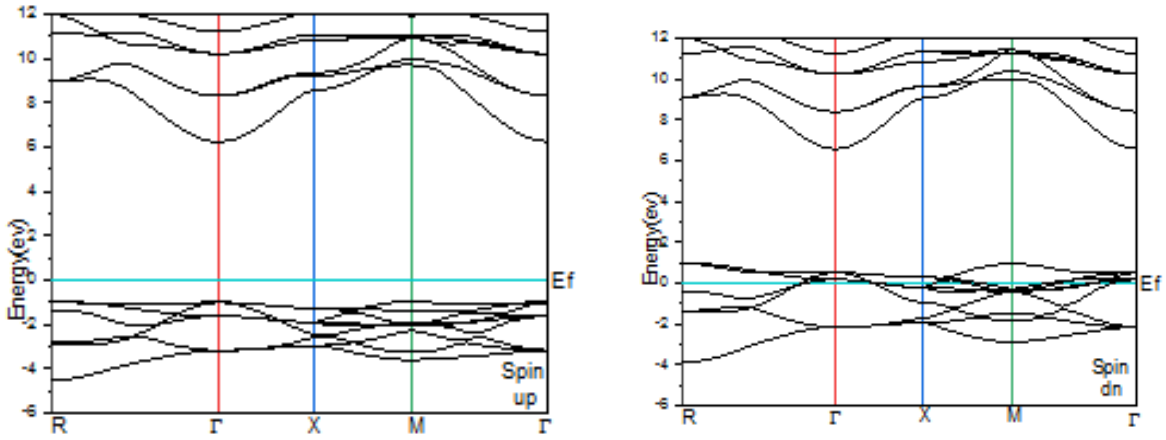

Fig2: band structure of $KMgO_3$ compound in both spin-up and spin-down states

CONCLUSION:

we used the FP-LAPW method founded in the DFT to calculate the different parameters of $KMgO_3$. Calculations reveal that the compound $KMgO_3$ has a minimum energy in ferromagnetic configuration. According to results of elastic properties, we found that our material KMgO3 shows ductile behavior and suggests a high metallic nature like inter-atomic bond. For electronic properties, it is clear that the material has a half-metallic character, this type of material can be very interesting for future spintronics applications.

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