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Enhancement of the magneto-electronic properties by GGA and TB-mBJ approaches for $KMgO_3$ perovskite oxide

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Abstract

we investigate the structural, elastic, electronic and magnetic properties of $KMgO_3$. First-principal calculations, based on the formalism of the density functional theory (DFT) and the method of full potential augmented and linearized plane waves (FP-LAPW) implemented in the Wien2k code. The exchange and correlation effects were treated by the following two approximations: generalized gradient approximation (GGA) and Tran-Blaha modified beck Johnson (TB-mBJ) potentials. After analyzing the obtained structural parameters, the results revealed that $KMgO_3$compound is most stable in its ferromagnetic configuration. The formation energy value showed that this compound can be experimentally synthesized. Furthermore, the calculated band structures, and density of states (DOSs) indicate the half-metallic behavior of $KMgO_3$. We found also that the total magnetic moment is an integer value of 3μBwhich confirms the half-metallic character. The magnetic moment specially issues from the spin-polarization of p electrons of O atoms.

Keywords: *$KMgO_3$; FP-LAPW; perovskite; half metallicity, ferromagnetic*

1. Introduction

Much effort has been spent to comprehend, forecast and grow new half metallic material. During the last decades, the HMF used in spintronics technology was based exclusively on transition metals. The latter have an electronic filling up to the d or f orbital [1]; and it is precisely these electrons which are at the origin of the magnetism and of the HMF in the materials based on these elements. In contrast, recent research, theoretical and experimental, has revealed the existence of magnetism in materials involving light elements such as alkali and alkaline earth metals [2-4] such as LiBeO3 and KBeO3 [5, 6]. Used with carbon, nitrogen or oxygen, these materials have been predicted to be excellent HMF, the origin of which is no longer linked to d or f electrons as in transition metals, but to s and p electrons of these three elements. In this case the simple perovskite, not including transition elements are very promising candidates.

This is what motivated us to suggest a study of $KMgO_3$ in the cubic phase, using ab-initio simulation studies [7], within the framework of the DFT according to the wien2k code [8]with a systematic study of the structural, elastic, magnetic and electronic properties. This paper is organized as follows: after the introduction, insection2, we described the employed method. Discussion of the results obtained in the present work will be presented in section3. Finally, we will end this study with a general conclusion.

2. Computational method

In this study, we calculate the structural, elastic, and magneto-electronic properties of perovskite oxide KMgO3, using the Full Potential Linear Augmented Plane Wave (FP-LAPW), implemented in the code WIEN2k [8] and within the density functional theory (DFT) [9, 10].The exchange and correlation effects were treated by the following two approximations:

generalized gradient approximation (GGA) [11] and Tran-Blaha modified beck Johnson (TB-mBJ) potentials [12],the plane wave cut-off value RmtKmax = 8 is used. The radius of the Muffin-Tin sphere (RMT) was chosen to be 1.94, 1.74and 1.33, for K, Mg and O, respectively. The Taken maximum angular momentum value, inside MT spheres for the expansion of wave functions, is Lmax=10 and Gmax= 14 Ry1/2.The convergence criteria for the integrated charge and energy differences between successive iterations are set to less than 10-4e and 10-5Ry, respectively.

3. Results and discussions

This part describes and discusses the structural, elastic, electronic and magnetic properties of $KMgO_3$.

3.1. Structural properties

As mentioned above, our considered material is the perovskite oxide $KMgO_3$.Therefore, it is investigated in the cubic structure with the Pm3m(221) space group, where the positions of the atoms are K (0, 0,0),O(0,0.5,0.5) and Mg(0.5,0.5,0.5),seefigure1.

In order to obtain the structural ground state of our study compound, we have performed the calculations, using GGA [11], of the total energy as function of volume for

its ferromagnetic (FM), non-magnetic (NM), and antiferromagnetic (AFM) phases. The equilibrium lattice parameter, bulk modulus B and its derivative B' are determined by fitting the curve of the total energy as a function of volume to the Birch-Murnaghan equation[13], given by the following equation:

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 \grave{B}_0 + \left[\left(\frac{V_0}{V}\right)^{`2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \quad (1)$$

Where E_0 is the equilibrium total energy, V_0 is the volume of the unit cell at zero pressure, B_0 and B_0'arethebulkmodulusanditspressurederivative, respectively.

The E (V) curves are illustrated in figure 2. From this figure, it clear that our compound is more stable energetically in its FM phase. We find the ground-state parameters (a_0, Band B '), as shown in table 1.

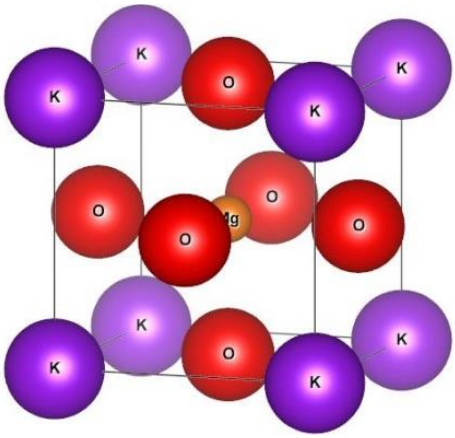


Figure 1: unit cell of KMgO3

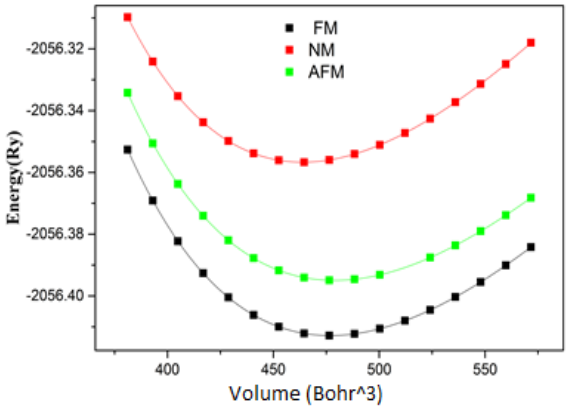


Figure 2: Calculated total energy of $KMgO_3$ compound as a function of the volume.

Table 1: Calculated values of the lattice parameter (Å), bulk modulus (GPa), its pressure derivative and ground state energies (Ry) for FM, NM, and AFM phases of $KMgO_3$.

Phase	a0	B	B’	Emin
FM	4.1344	61.7614	4.3491	-2056.41281
NM	4.0964	65.8905	4.3618	-2056.35667
AFM	4.9287	59.8364	4.2946	2056.394958

3.2.Elastic properties

To investigate the mechanical stability of our compounds, the calculation of the elastic constants using IRelast package, integrated in the WIEN2k code is performed. The elastic properties give various kinds of important information, on the behavior of this compound in addition to the ductility, brittleness and application of the external forces.

The mechanical stability of a cubic system requires that Born’s stability criteria should be met [14]:$C_{44} > 0$, $C_{11} - |C_{12}| > 0$, $C_{11} + 2C_{12} > 0$ and $C_{12} < B < C_{11}$, ,which reflects the stability of our material in this structure against elastic deformations. The calculations of elastic constants are performed, using the energy-strain approach implemented in theWIEN2k code [8], for the energetically favorable phase.

According to Born's stability criteria, our compound is found to be mechanically stable in this phase. Other quantities related to the elastic constants can be deduced, such as the shear modulus G, the Young's modulus E, the anisotropic parameter A, the ratio B/G and the Poisson's ratio ν. The obtained B/G ratio value of our material is higher than the critical value 1.75 which separates the ductile / brittle (brittle <1.75< ductile) behavior [15], as mentioned in table2.Accordingly,ourcompoundcanbeclassifiedas a ductile material. As can be seen from table 2, the anisotropic parameter A is smaller than 1. Thus, KMgO3 exhibits an anisotropic character.

To further confirm the stability of this compound, we calculated the formation energy, in order to examine the thermodynamic stability related to its synthesizability. The formation enthalpy can be computed by given equation.

$$E_{Formation}^{KMgO3} = E_{Total}^{KMgO3} - \left(E_{bulk}^{K} + E_{bulk}^{Mg} + 3/2\, E_{bulk}^{O2}\right) \quad (2)$$

The obtained negative formation energy of -0.075 Ry indicates that $KMgO_3$ is thermodynamically stable. Therefore, it can be synthesized in the normal conditions.

Table 2. Calculated elastic constants C11, C12, and C44, bulk modulus B,shear modulus Gand Young's modulus E(in GPa). Poisson's ratio ν, Zener anisotropy factor A, B/G ratioand Debye temperature (θD in K) for $KMgO_3$.

C_{11}	C_{12}	C_{44}	B	G	E	ν	B/G	A	θ_D
121.5406	32.5717	9.0363	62.228	23.21556	49.846	.366	2.68044	0.2031	366.264

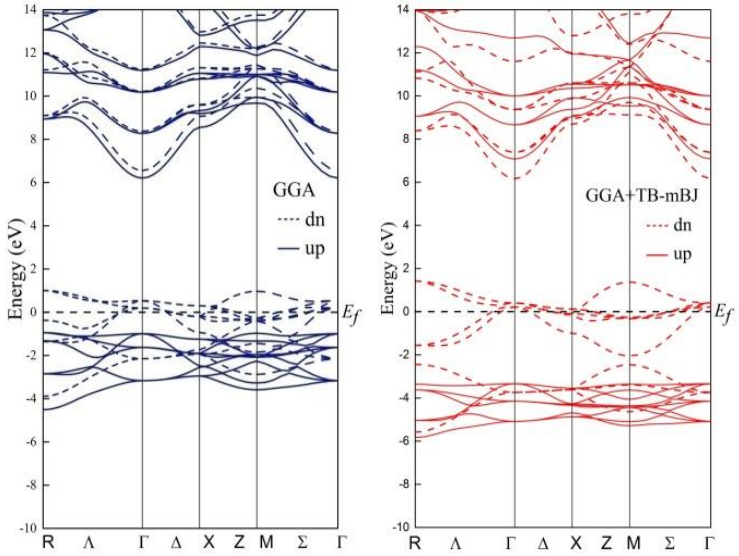
3.3.Electronic properties

The following electronic properties are inspected at equilibrium lattice constants using GGA method. Furthermore, it is extended to TB-mBJ potential in order to more precisely describe the electron profile and results are discussed.

3.3.1. Band structures

From the plots in Figure. 3, We notice that the curves show a gap separating the valance and the conduction bands in majority spin directions (spin-up); whereas the minority spin states (spin –dn) are strongly metallic with bands crossing Fermi level.

From GGA method, there is an indirect gap R-Γ of 7.15 eVand the half-metallic gap is found to be 0.99 eV. These electronic results confirm the half-metallic property with full spin polarization (P = 100%) of this cubic oxide perovskite. On using TB-mBJ potential, the band gap and half-metallic gap in spin-up state of our studied compoundis increased. This method offers a wide indirect band gap of 10.41 eV with VBM at R-point and CBM at Γ-point, while the observed HM gap of 3.33 eV. Also, The TB- mBJ band structure proved half metallic character.



(a) (b)

Figure 3: spin resolved band structure of $KMgO_3$

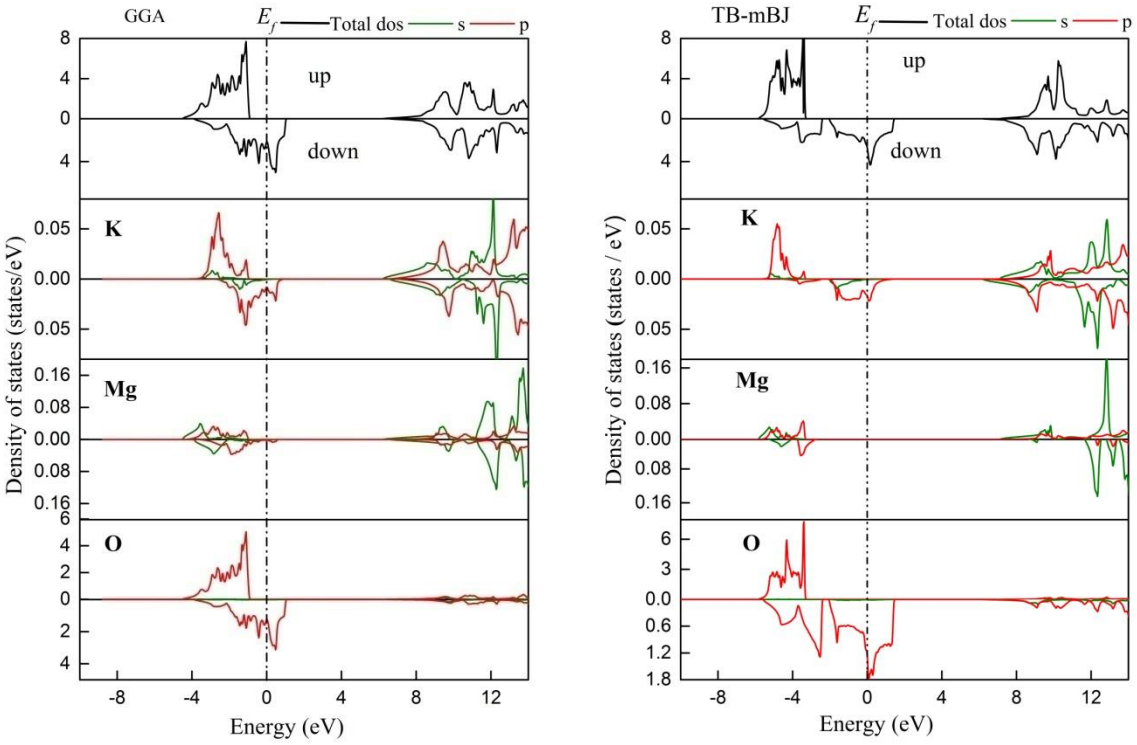
by:**(a).** GGA;(b) GGA+TB-mBJ approximation. (Dash line for spin down and solid line for spin up).

3.3.1. Densities of electronic states

In order to give a deep insight on the origin of the half metallic character, the total and partial densities of states of this compound are calculated and given in Figure.4

The TDOSs confirm the half-metallic nature of our compound in both level of theory GGA and TB-mBJ.

The PDOSs show that spin exchange splitting is fundamentally originated from p states of oxygen (O) atoms in both approaches (GGA and TB-mBJ). Around Fermi level, there are no contributions of Mg. But p states of K have a little contribution in both spin channels.



(a) (b)

Figure 4: Calculated DOS of $KMgO_3$ compound in both spin-up and spin-down states by: (a). GGA; ((b). GGA+TB-mBJ approximation.

3.4. Magnetic properties

In this section, we begin to understand the magnetic character of $KMgO_3$ compound. As shown in table 3,the magnetic character comes mainly from O atoms and the main contribution to the magnetic character in the resulting DOS, obtained by the GGA and GGA+TB-mBJ methods around the Fermi level, is due to the orbital p of O atoms. It is found that O has a larger magnetic moment. This result is confirmed by the results of the DOS (figure 4). The total magnetic moment of our studied compound has the integervalue of 3μB.

Table 3: Calculated total, partial, and interstitial magnetic moments (in μB) in the unit cell for $KMgO_3$.

Method	Mtot	MK	MMg	MO	Mint
GGA	3.000	0.001	-0.008	0.726	0.830
TB-mBJ	3.000	0.002	-0.023	0.902	0.314

4. Conclusion

The investigation of the structural, elastic, electronic and magnetic properties for $KMgO_3$ perovskite is performed, applying the FP-LAPW method. The calculations show that its ferromagnetic state is more stable than non-magnetic and anti-ferromagnetic phases. The electronic band structures indicate that $KMgO_3$ has a half-metallic character with a large band gap of 7.15 eV and 10.41eV for GGA and TB-mBJ methods, respectively, in the spin-up channel, at the B → Γ direction. This half metallicity is mainly resulted from spin polarization of O-p orbitals in both approaches. The total magnetic moment is found to be an integer value of 3 μB, which point also out the half-metallic character. The most interesting aspect of our work is that O-p orbital is responsible of half-metallic behavior for the perovskite $KMgO_3$.

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