First principle calculation studies of half-metallic ferromagnetism in Au-doped MgO

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Abstract

On the basis of first principles calculation, the structural and electronic properties of Au doped MgO are investigated using generalized gradient approximation (GGA) method within the framework of density functional theory (DFT). Transition metal Au is doped in the host compound of MgO in a doping concentration of 12.5% by replacing the Mg atom to form the compound $Au_{0.125}Mg_{0.875}O$. The volume optimization was carried out for both magnetic and non-magnetic phases of $Au_{0.125}Mg_{0.875}O$ to determine the equilibrium energy and lattice constant. $Au_{0.125}Mg_{0.875}O$ is found to be more stable in the ferromagnetic phase than in non-ferromagnetic phase. The DOS and band structure of the compound $Au_{0.125}Mg_{0.875}O$ shows a wide band gap at Fermi level (E_F) in the majority spin channel whereas in the minority spin channel the compound exhibits metallic character. The wide band gap in spin up direction confirms the half-metallic ferromagnetic (HMF) property of the compound $Au_{0.125}Mg_{0.875}O$.

Keywords: ***MgO; First-principles calculations; Half-metallic ferromagnetism; structural property; Electronic property.***

1. Introduction

The aim of this work is to investigate the structural and electronic properties of MgO doped with 4d transition metal (Au). MgO is an insulator with a band gap of 5 eV which on doped with the impurities changes its properties. Ferromagnetism has been reported on doping of transition metals in MgO [1]. Electronic, magnetic and optical properties were predicted on doping MgO with transition metals [2, 3]. Ferromagnetism also produces when MgO is doped with non-metals like carbon, nitrogen [4, 5]. Half-metallic ferromagnetism has been predicted in MgO when it is doped with the transition as well as non-metals [2, 6]. Half-metallic ferromagnetism was first predicted in some Heusler alloys in 1983 [7, 8]. It is known that Half-metallic Ferromagnetic materials are best candidates for spintronic applications. These materials have one majority spin channel semiconducting while other minority spins channel conducting or vice versa and hence expecting 100% spin polarization at Fermi level.

In this work, the investigation of half-metallic ferromagnetic was observed in MgO doped with gold (Au). The resulting compound $Au_{0.125}Mg_{0.875}O$ exhibit the half-metallic character leaving a band gap at Fermi level in majority spin state.

2. Method of Calculation

A spin-polarized Full Potential Linear Augmented Plane Wave method was used for the First principles calculations within the framework of density functional theory [9, 10]. The electronic properties were studied using WIEN2k code [11, 12] which employs the full potential linearised augmented plane wave plus local orbitals. In the FP-LAPW+lo method, the spherical harmonic expansion was used, inside non-overlapping muffin-tin (MT) spheres and plane waves in the interstitial region with cut-off RK_{MAX} =7. And this method is proven to be an accurate method as implemented in the WIEN2k

package for computation the structural, electronic and magnetic properties [13]. The energy cut was chosen as -8 Ry for defining the separation of states.

The supercell was constructed for studying electronic properties of Au doped MgO. The doped MgO was modeled in 2×2×2 supercell consisting of 16 atoms (8 Mg atoms and 8 oxygen atoms) in rock salt phase. When Au is doped to host compound to replace Mg with doping concentration x=0.125 and remaining atoms are at their specified positions. The primitive unit cell of MgO has NaCl rock salt structure belongs to cubic (Fm3m) space group with lattice constant equal to 4.21 Å. The numbers of k-points in the whole Brillouin zone are chosen as 63 k-points and total energy of the crystal converges to less than 10^{-4} Ry.

3. Results and Discussion

3.1. Electronic structure

MgO has the rock salt structure with space group 225 (Fm3m) and position of atoms as Mg (0,0,0) and O (½,½,½). One impurity atom is doped into the host compound MgO. The supercell is formed after replacing the Mg atom by Au. Au is doped in MgO compound to investigate the changes in the structural and electronic properties of MgO. The crystal structure of $Au_{0.125}Mg_{0.875}O$ compound is plotted as shown in Figure 2 using the Vesta software [14]. The volume optimization for the compound was carried out in GGA method as shown in Figure 1. The compound $Au_{0.125}Mg_{0.875}O$ is found to be stable in ferromagnetic phase. The equilibrium energy was observed after volume optimization and lattice constant was calculated is shown in Table 1.

Table 1. Minimum Equilibrium energy and lattice constant of doped compound

S.N	Compound	Phase	Equilibrium Energy (Ry)	Lattice constant (Å)
1	$Au_{0.125}Mg_{0.875}O$	Ferromagnetic	-42105.872288	8.81
		Non-magnetic	-42105.869305	8.81

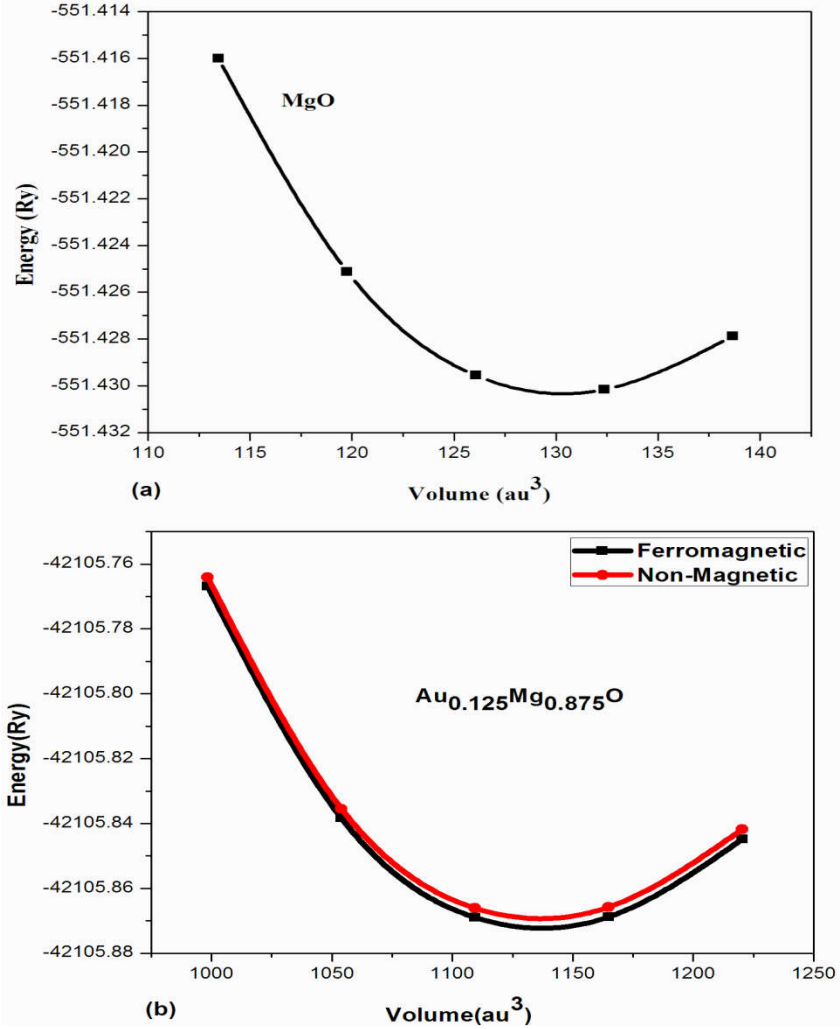

Figure 1. Volume optimization curves of (a) MgO (b) $Au_{0.125}Mg_{0.875}O$

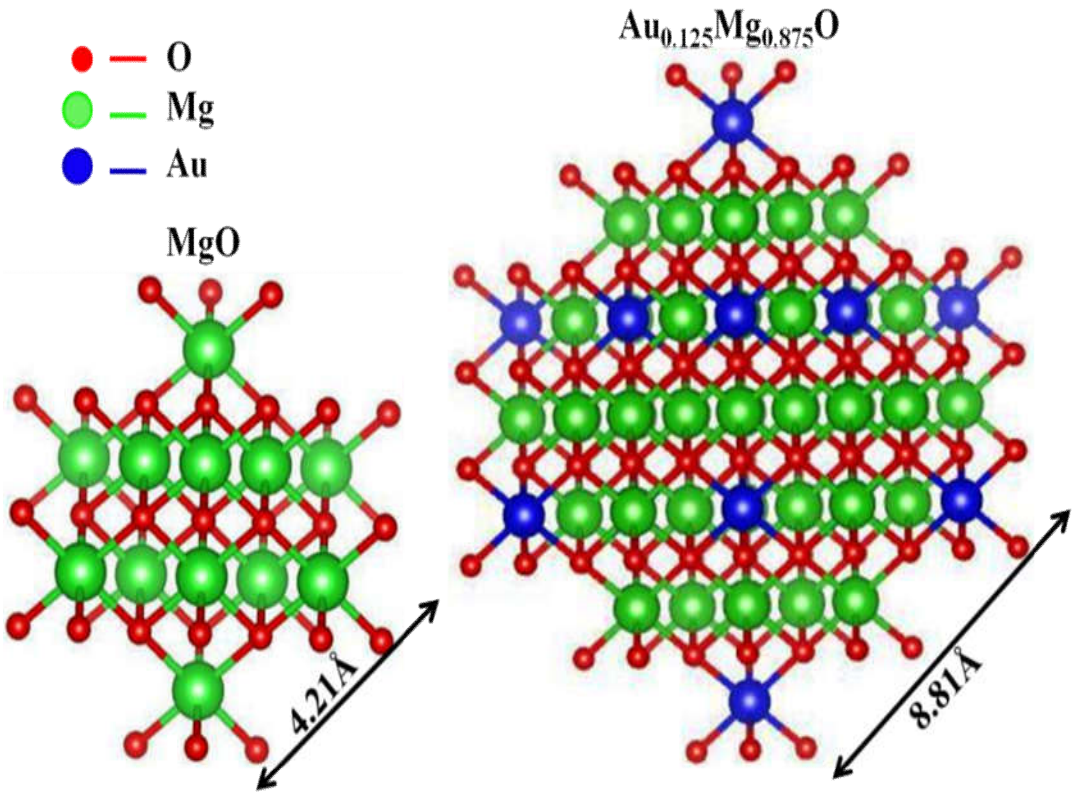

Figure 2. Crystal structure of (a) MgO (b) $Au_{0.125}Mg_{0.875}$

3.2. Half-metallic property

Half-metallic property is that in which one spin is occupied by electronic states and other is empty at the Fermi level. On substitution of Au in the host compound MgO, it is investigated that the resulting compound shows the half-metallic ferromagnetism. The lattice constant equal to 4.21 Å was used to calculate the density of states and band structure. The electronic properties of MgO compound with doped 5d transition metal (Au) were investigated. The total DOS, partial dos and band structure of $Au_{0.125}Mg_{0.875}O$ compound are shown in Figure 3and 4. The compound $Au_{0.125}Mg_{0.875}O$ shows the semiconductor behavior in spin up direction and metallic nature in spin down direction. *Au-d* bands at the Fermi level in majority spin are not crossing the Fermi level but are pushed each other making a band gap equal to 0.85 Å.The band gap is measured between the energy bands (conduction and valence bands) at the Γ point. From partial dos, it is clearly visible that the whole contributions of Au-d bands are responsible for creating the band gap at Fermi level and in minority spin, the Au-d bands cross the Fermi level and confirm the metallic character. Therefore, the compound $Au_{0.125}Mg_{0.875}O$ shows semiconductor character in majority spin channel and metallic character in minority spin channel which explains half-metallic ferromagnetism.

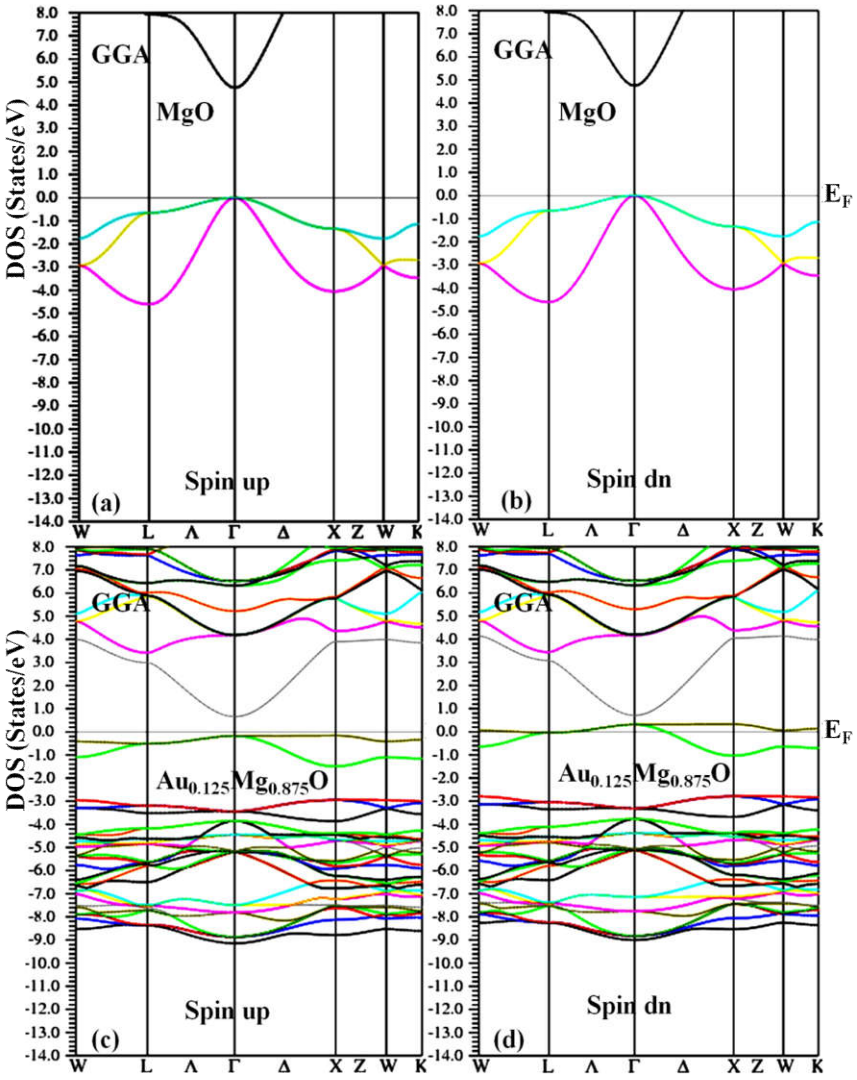

Figure 3. Band structures of MgO and $Au_{0.125}Mg_{0.875}O$

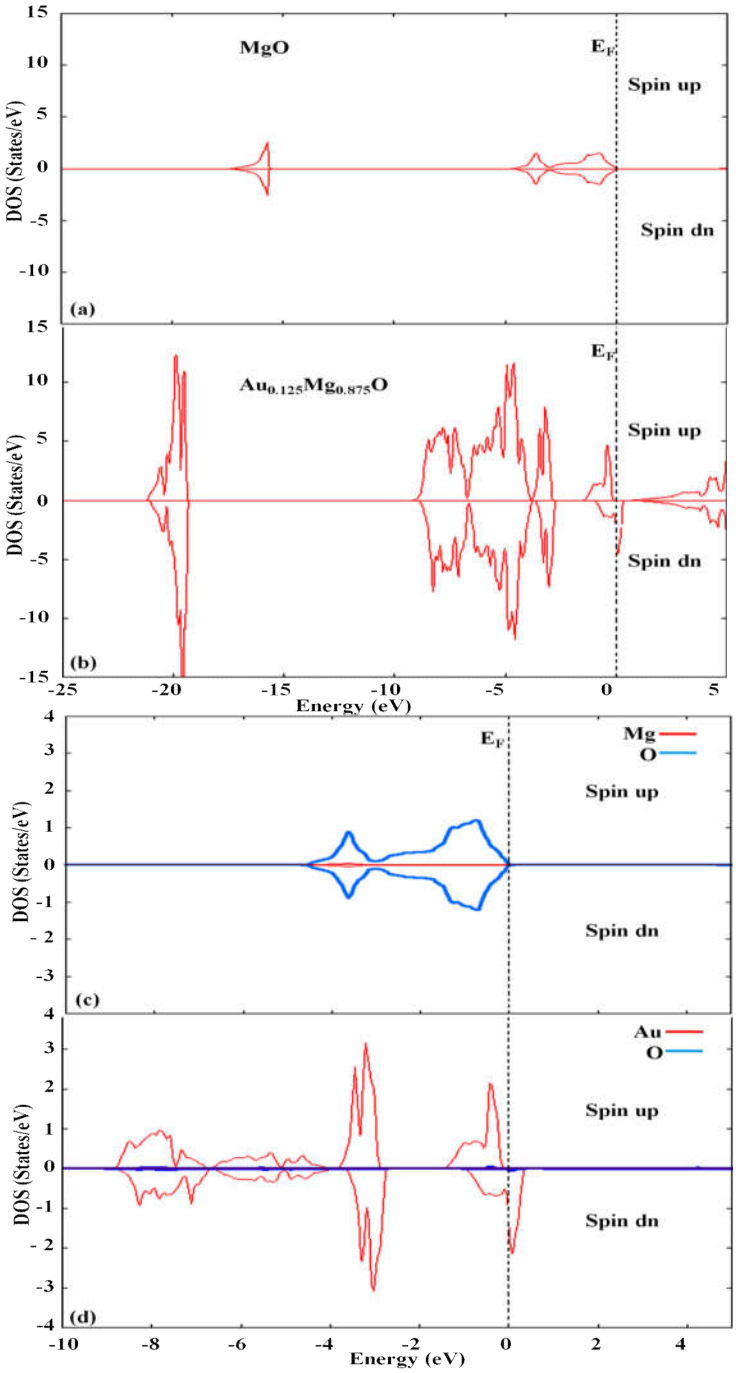

Figure 4. Total dos of (a) MgO (b) $Au_{0.125}Mg_{0.875}O$ and Partial dos of (c) MgO (d) $Au_{0.125}Mg_{0.875}O$

4. Conclusion

The electronic structures and half-metallic ferromagnetic properties were investigated by the first-principles method. The doping of transition metal atom changes the electronic properties of magnesium oxide and it is predicted that the compound exhibits half-metallic ferromagnetism. It is observed that doping atom fully contributes in performing the band gap at Fermi level. There is no role of oxygen and

magnesium atoms in creating the band gap only the bands seen in partial dos are 5-d Au bands. The Dos and the band structure show the half-metallic character of the compound $Au_{0.125}Mg_{0.875}O$.

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