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Half-metallic ferromagnetism in Fe and Co doped cubic Zinc Oxide: Theoretical investigation of electronic, ground-state and magnetic properties

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Abstract: First principle calculations within the density functional theory was used to investigate the possibility of existence of half-metallic ferromagnetism in Fe and Co doped ZnO compounds. First, the calculations were performed to study the electronic and ground-state properties of parent ZnO compound in zinc blende type structure. The result of the calculation shows that the ZnO is a direct band gap semiconductor with a band gap equal to 0.60 eV at ambient conditions. By interchanging the position of the atoms in cubic ZB-type structure there forms new phases. The spin polarization calculation shows that these compounds are more stable in ferromagnetic phase at their equilibrium and expanded volume. The calculations reveal that the doped atoms can induce the ferromagnetism and half–metallicity. In these compounds, the magnetic moments is mainly comes from the doped atoms and it may be used in spintronic devices.
Keywords: Half-metallic materials, Total energy, first-principles calculations, diluted magnetic semiconductors.

1. Introduction

Dilute magnetic semiconductors are recently very attractive subject of current researches, where the manipulation of the electron spin and charge can give rise to new electronic devices [1]. As one of the most important wide-band-gap oxides, ZnO has received considerable interest for its variety of applications in industry. The room temperature ferromagnetism was reported by Dietl et al. (2000) in Mn-doped ZnO [2]. After that, many researchers have studied doped ZnO with 3d transition metal and reported room temperature ferromagnetism [3]. In the present work, we explored the electronic and magnetic properties of ZnO doped with VIII ions (Fe and Co) based on first-principles calculations. For this purpose, we have used the Interstitial Insertion Rule. This study provides us with an understanding of the novel properties of doped ZnO materials which is essential to employ Fe and Co doped ZnO as building blocks for the electronic devices.

2. Crystal Structure and Methodology

The structural details for Fe and Co doped ZnO compounds are as follows: In zinc-blende type related structure, $A^{I}B^{II}C^{V}$ compounds may be viewed as follows: D^{III}-C^{V} compound in zinc-blende structure has the D^{III} atom at the sublattices. One could transmute D^{III} atom into its iso-valent pair A^{I}+B^{II} by inserting a closed shell

atom in one of the empty sites and distribute these among the sublattices. It is called as the Interstitial Insertion Rule [4]. There are three distinct ways of distributing periodically three atoms A, B, C on the four sublattices τ_1, τ_2, τ_3 and τ_4 and the resultant structures are denoted as α- (ZnOTM), β- (ZnO TM) and γ- (TMO Zn) phases of the cubic-$A^IB^{II}C^V$ compounds. The symbol means a vacant site and technically in connection with the LMTO method an "empty sphere". The cubic γ-phase is also denoted as MgAgAs (ordered CaF_2)-type structure (Galasso 1970) [5]. The present calculations are based on the density functional theory [6]. The von Barth and Hedin spin polarized exchange correlation potential is used in the local spin density functional approximation. The tight binding linear muffin-tin orbital (TB-LMTO-ASA) method was employed [7]. The maximum overlaps between the spheres have been approximately kept at 16%. The density of states was calculated by the tetrahedron method [8]. We use 512 **k**-points in the irreducible part of the Brillouin zone to construct the tetrahedrons. E and **k** convergence are also checked.

3. Results and Discussion

3.1 Total energy calculation and ground state properties

Both spin-polarization and non-spin-polarization calculations have been performed for the Fe and Co doped ZnO compounds in the ordered MgAgAs-type structure. The total energy as a function of molecular volume was calculated for these compounds. The calculation shows clearly that the Fe and Co doped ZnO compounds have lower energies in the ferromagnetic (FM) phase when compared with the nonmagnetic (NM) phase. The cell parameter values are optimized using the cell parameter values of ZnO. The calculated equilibrium lattice parameters (a_0)and bulk modulus (B_0) and its pressure derivatives (B_0') of these compounds were estimated by fitting the total energies to the Birch equation of state. From the Table 1, it is observed that these compounds have large lattice constant compared to parent ZnO. It is due to the fact that, at anion (O) atoms are rather closer to the neighboring cation atoms (Zn, TM) as compared to anion atoms (O) at ZnO. Parent ZnO has a smaller cell volume and a higher bulk modulus, indicating that the bonding is stronger due to the smaller interatomic distance.

Table 1: Calculated parameters in FM and NM phases at their equilibrium volume

Compounds	Phase		a_0 in Å	B_0 in GPa	B_0'	Wigner-Seitz radius, S_0 in Å	E_g in eV
ZnO	NM	Present	4.612	142.441	4.448	1.139	0.600
		Others [5, 9, 10]	4.616, 4.627, 4.633, 4.504, 4.62	125.34, 131.60, 133.73, 135.30, 160.80	3.44, 3.33, 4.79, 3.70, 5.70	-	0.55, 0.60 0.65, 1.46 0.58
ZnFeO	FM		5.320	117.301	4.822	1.310	-
	NM		5.310	129.482	4.525	1.310	-
ZnCoO	FM		5.220	129.550	4.074	1.285	-
	NM		5.167	133.205	4.091	1.285	-

3.2 Electronic band structure and density of states

The self-consistent relativistic spin-dependent electronic band structure for titled compounds is obtained using spin-polarized and non-spin-polarized calculations within the LDA along the high-symmetry directions. The spin-polarization calculations show that these two compounds are ferromagnets at their equilibrium and expanded volume. The calculation shows that the majority and minority spin channels are metallic in nature at their equilibrium volume. The overall band structure profiles for these two compounds are similar. In these compounds, the bond formation occurs from the doped cation s-like electrons and anion p-like electrons. However, the magnetism arises mainly due to the doped cation d-like electrons. The doped cation d-like states are strongly spin-split i.e. strongly spin polarized and is situated close to the Fermi level. The magnetic moments of these compounds originates mainly from the d-electrons of the doped cation. The calculated magnetic moments for these compounds are given in Table 2 along with partial magnetic moments at each atomic site. Their magnetic moments are small around the equilibrium volume when compared with expansion of volume. From the Table 2, it can be seen that the main contribution to the magnetic moments comes from the doped cation d-electrons. A very small contribution to the magnetic moment comes from the parent cation Zn, anion O and interstitial site.

Table 2: Calculated total and partial magnetic moments (μ) in μ_B

	Compounds	a_{hm}	Magnetic moments				
			Cation		Anion	Empty	Total
			Fe/Co	Zn			
Equilibrium Volume	**ZnFeO**	-	2.535	0.013	0.098	0.029	2.616
	ZnCoO	-	1.330	0.019	0.143	0.032	1.421
Half-metallic Volume	**ZnFeO**	6.173	3.448	0.103	0.445	0.004	**4.00**
	ZnCoO	6.619	2.278	0.064	0.656	0.002	**3.00**

Figure 1 shows that the spin-dependent calculation of the electronic band structures for MgAgAs-type ZnFeO and ZnCoO compounds at their half-metallic or critical volume. From the figures one can easily observe that these compounds exhibit half-metallicity (HM). This is obvious that the majority spin bands are metallic nature but the Fermi level is situated within very small energy gap for the minority spin bands. The half-metallic lattice constant, total and partial magnetic moments are given Table 2. An integer value of magnetic moment is a characteristic feature of HM ferromagnets.

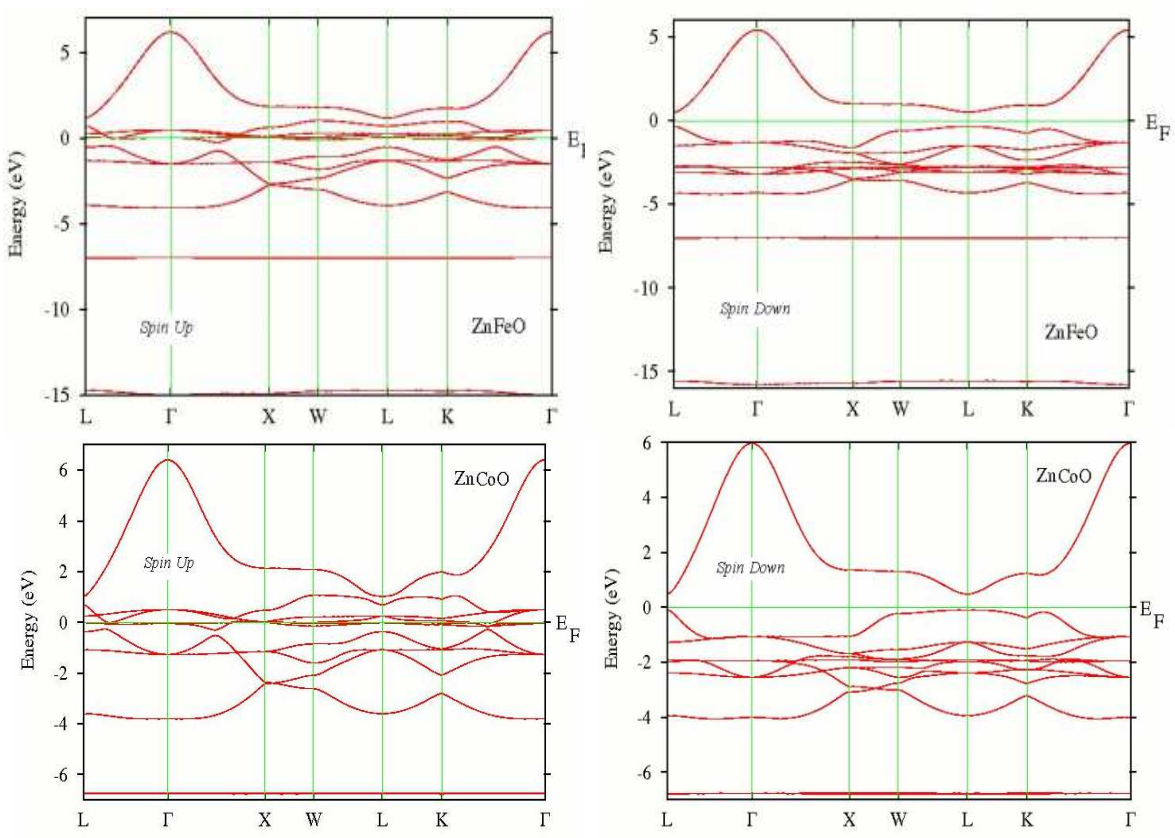

Figure 1: Spin-dependent electronic band structures of ZnFeO and ZnCoO at their half-metallic volume.

4. Conclusion

The spin-polarization calculation shows that these two compounds exhibit ferromagnetic property with small magnetic moment at their equilibrium volume. However, these compounds exhibit half-metallic ferromagnetism with the integer magnetic moments as expected under large volume expansion. In these compounds, unit cell volume plays an important role in exhibiting half-metallicity. The magnetism arises mainly from the doped cation d-like states.

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