Journal of Magnetism and Magnetic Materials 419 (2016) 233–239

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Theoretical investigation of electronic, magnetic and optical properties of ZnSe doped TM and co-doped with MnTM (TM: Fe, Cr, Co): AB-initio study

M. Behloul [a], E. Salmani [a,*], H. Ez-Zahraouy [a], A. Benyoussef [a,b]

[a] LMPHE (URAC 12), Departement of Physique, B.P. 1014, Faculty of Science, University Mohammed V, Rabat, Morocco
[b] The Institute for Nanomaterials and Nanotechnology, MAScIR (Moroccan Fondation for Advanced Science, Innovation and Research), Rabat, Morocco

ARTICLE INFO

Article history:
Received 24 November 2015
Received in revised form
1 June 2016
Accepted 8 June 2016
Available online 10 June 2016

Keywords:
Spintonic
Ferromagnetism
ZnSe
AB initio calculations
absorption

ABSTRACT

Based upon the first principal spin density functional calculation, the electronic, magnetic and optical properties of ZnTMSe and ZnMnTMSe where TM=Fe, Cr, Co are studied using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method within the local density (LDA)and the self-interaction-corrected(SIC) approximation. The purpose of this study is to determine the effect of different type of dopant and concentration on ferromagnetic and half metallic behavior of ZnSe. Therefore the magnetic disorder local moment (DLM) and the ferromagnetic state are investigated for different concentrations of Mn, Fe, Cr and Co; also the advantages of co-doped ZnSe with TM elements, behavior at room temperature are discussed. The electronic structure and optical properties are studied employing the local density (LDA) and the self-interaction-corrected (SIC) approximation. Moreover, the X-ray spectra modeling are in good agreement with the electronic and magnetic properties results.

1. Introduction

Diluted magnetic semiconductors (DMS's) will play an important role in spintronics as semiconductors do in electronics because of their easy integration into existing electronic devices [1]. The DMS's are characterized also by some degree of the magnetic disorder [2], their interesting behavior as metals in a one spin channel and as insulators in the other [3]. Technological and theoretical interest in II–VI compounds and their alloys in either wurtzite or zinc-blende structures have been growing recently due to its appealing properties in med-IR sources blue-green diode lasers, electro-optical, electro-acoustic devices [4,5] solar cells and optically controlled switching due to its low absorptivity at infrared wavelength, visible transition and giant photoresistivity [6]. ZnSe and II–VI semiconductors in general, may be used for the realization of diluted magnetic semiconductors have ferromagnetic, anti-ferromagnetic properties or according to the nature of the dopant [7], for applications in the spintronics field. In DMS materials, transition metal (TM) or rare earth metal ions are substituted onto cation sites of the host semiconductor and coupled with free carriers to introduce ferromagnetism [8]. Furthermore, in recent years ZnSe has proved to be a particularly interesting dilute magnetic semiconductor when doped with Mn [9].

Transition metals (TM) doped ZnSe have attracted large research interest as new, efficient device materials [10], with the possibility of being used as microelectronic magnetic when doped with a variety of 3d transition metal ions such as Mn [11], Co [12], Cu [13] Fe [14] and Cr [15]. The recent studied of these compounds show that, MnZnSe and CuZnSe could be used in spintronic devices only if additional dopants are introduced; on the contrary, CrZnSe, FeZnSe and CoZnSe [10]which showed delocalized quality and might be promising half-metallic and ferromagnetic materials for applications in spintronics. Moreover, a few studies of doped ZnSe with single and double TMs for lower concentrations are known.

The development of new generation spintronic devices requires new semiconductor materials having ferromagnetism at room temperature.

Important technique which influences strongly the magnetic properties of semiconductor materials is co-doping. Co-doping is a fairly simple and effective method to alter the number of vacancies and interstitial host metal atoms, which is useful to explore the mechanism of ferromagnetism at room temperature [16]. Recently, we have been proposed materials, design of the co-doping method for the realization of low resistivity p-type wide band gap semiconductors such as GaN [17], ZnSe [18] and AlN [19], based on the analysis on a change in the lattice energy and electronic structures

* Corresponding author.
E-mail addresses: elmehdisalmani@gmail.com, salmanielmehdi@gmail.com (E. Salmani).

http://dx.doi.org/10.1016/j.jmmm.2016.06.011
0304-8853/

by the co-doping. In our calculation, we have chosen Mn as co-doping element because it has a relatively large magnetic moment (S=5/2), characteristic due to half filled 3d bands; and it is possible to incorporate in large amounts in the host matrix without affecting the crystallographic quality of the final material [3], thus avoiding the formation of any acceptor or donor impurities in the crystal.

The aim of this present work is to study the magnetic and electronic effect of doped and co-doping ZnSe with different concentration of single and double TM impurities (Mn, Fe),(Mn, Cr) and (Mn, Co), in order to assist in the choice of the applicant materials for practical application. On the other hand, we investigate the electronic and optical properties of $Zn_{0.90}Mn_{0.05}Cr_{0.05}Se$ with LDA and LDA-SIC approximation.

2. Calculation method

The electronic and magnetic properties of doped and co-doped Zinc selenide based on the Korringa-Kohn-Rostoker coherent potential approximation and local density approximation (KKR-CPA-LDA) method [20], have been studied, with the parameterization proposed by Moruzzi, Janak and Williams (mjw).

In our simulation, the self-interaction-correction is implemented into the package MACHIKANEYAMA2002 coded by Akai [21] as the basis set in KKR-CPA, within the muffin-tin spheres. The LDA-SIC approximation can be estimated as an extension of LDA, in the sense that the Kohn–Sham wave function is projected onto a set of localized orbital basis [22].

The relativistic effect is taken into consideration by the scalar relativistic approximation. The form of the potential is approximated by the muffin tin model. Moreover the wave functions in each muffin-tin sphere are expanded in real harmonics up to l=2, where l is the angular momentum quantum number of the respective sites. We have used the highest K-points up to 500.

In this paper the zinc blend structure is used for calculating, which belong to the F43M space group and their lattice parameter is a=b=c=5.667 Å [23] in spatial group of α=β=γ= 90, which predicts a direct band gap of 2.7 eV or bulk ZnSe at room temperature.

The unit cell contains two metal atoms (Zn) at position (0, 0, 0) and (1/4, 1/4, 1/4) for (Se). Each Zn atom (Se) is surrounded by four Se atoms (Zn) neighbors forming a perfectly regular tetrahedron.

3. Results and discussion

As seen in the diagram of electronic band structure of pure ZnSe within LDA and LDA-SIC approximation respectively the Fig. 1 indicate that, the band gap of ZnSe exhibit semiconductor character and has a direct band gap of Eg(LDA)= 1.6 eV within LDA and Eg(LDA-SIC)=2.5 eV within LDA-SIC, which is very close to the experimental value (2.7 eV). The difference between the value of Eg(LDA) and Eg(LDA-SIC) is due to the want of a discontinuity in this exchange correlation potential.

In order to further understand the changes of the electronic and magnetic properties of ZnSe, the total and partial densities of states (TDOS) and (PDOS) for $Zn_{1-x}Co_xSe$, $Zn_{1-x}Cr_xSe$ and $Zn_{1-x}Fe_xSe$ systems for x= 0.01; 0.03 and 0.05 have been calculated for LDA approximation (Fig. 2). In each case of Fig. 2(a, c, e, f, g and i) an impurity band appeared at the Fermi level originated from the 3d states of TM impurities, these impurities 3d bands are responsible for the magnetism of the system, therefore the impurity states show a large exchange splitting between spin up and down. This change in the band gap is due to the important hybridization between the band electrons and localized 3d electrons of TM's, called exchange interaction [24].

In particular, the half-metallic character is observed, except from the Fig. 2(b, d and h) where the Fermi level is situated at the top of the valence band (3d-Co) or in the middle of the majority spin states and minorities while the 3d-Cr impurity band is located at the top of the conduction band and the 3d-Fe impurity band is located near to the conduction band. In these last cases, both spin-up and spin-down are totally symmetric while the spin splitting is null. This means that these systems do not exhibit half-metallic or double exchange coupling behavior.

Furthermore the doped ZnSe with transition metals at 5% show stabilization in the ferromagnetic states. Moreover, beyond the 5% up to 25% the ferromagnetic state is stabilized by the double exchange mechanism for Cr, however the spin-glass state become stabilized as the atomic number of the TM increases. These results are in good agreement with the results obtained by Dietel and al [25] for the case of ZnSe doped single TM impurities. A similar behavior is reported for, ZnSe [26] ZnO, ZnTe and GaN [23].

To investigate the effect of introducing the Mn on the electronic properties, the total and local density of states of $Zn_{1-2x}Mn_xTM_xSe$ systems when TM (Co, Fe and Cr) for x=0.02, 0.03 and 0.05 respectively is shown in the Fig. 3. It is clear that for all compositions showing a half-metallic characteristic and 100% polarization at the Fermi level with a large exchange splitting between spin-up and

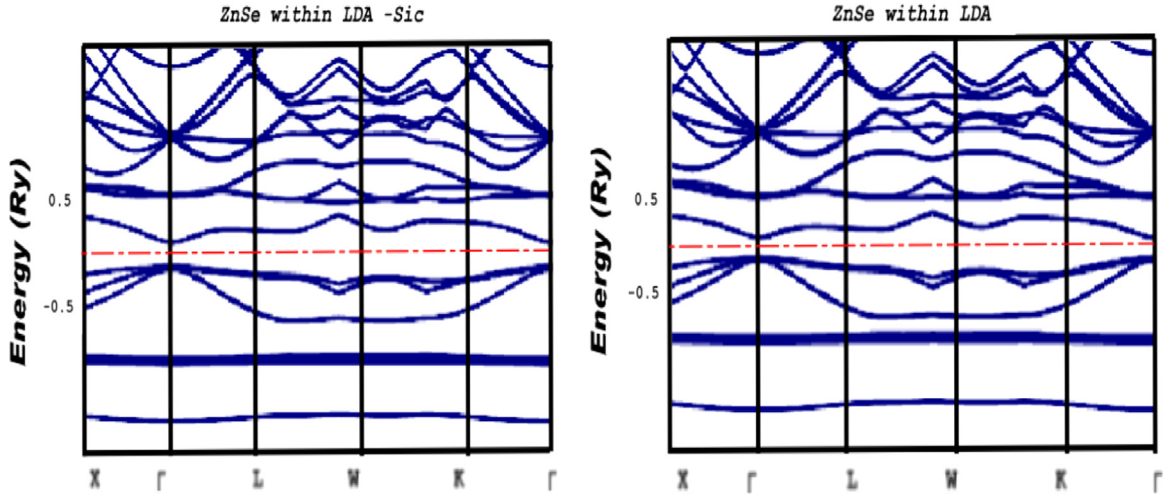

Fig. 1. The electronic band structure calculation of ZnSe within LDA and LDA-SIC approximation.