Journal of Magnetism and Magnetic Materials 446 (2018) 192–199

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Review Articles

Chromium and hydrogen doping effects on magnetic and electronic properties of ZnO

A. Larabi [a,*], M. Mebarki [a], A. Sari [b,c], G. Merad [b]

[a] Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE), Division DDCS, 2, Bd Frantz Fanon, BP 140 Alger 7- Merveilles, 16038, Algeria
[b] Division Etude et Prédiction des Matériaux, Unité de Recherche Matériaux et Energies Renouvelables, LEPM-URMER, Université de Tlemcen, Algeria
[c] Centre universitaire de Maghnia, Département des sciences et techniques, Tlemcen, Algeria

ARTICLE INFO

Article history:
Received 30 January 2017
Received in revised form 21 August 2017
Accepted 2 September 2017
Available online 18 September 2017

Keywords:
ZnO
Hydrogen
First principle calculations
DMS

ABSTRACT

The effect of Hydrogen insertion on the electronic and magnetic properties of the Cr doped ZnO has been investigated using the density functional theory DFT approach within the GGA and GGA+U methods. The electronic density of states (DOS) shows that the magnetic contribution appears to be n-type in H-ZnO. The calculated formation energy indicates that interstitial hydrogen atom prefers to bond with oxygen atom in the Cr—O bond center. Calculations show that the existence of interstitial hydrogen increases the local magnetic moment of Cr in $Zn_{1-x}Cr_xO$. The hydrogen implantation increases the magnetic moment in the CrZnO. Calculations are done for different doping concentrations to discuss the contribution of different atoms to the magnetic moments.

Contents

1. Introduction

ZnO is a wide-band-gap semiconductor, which crystallizes in hexagonal wurtzite, zincblende and rocksalt structures. However, due to its potential applications especially in the last decade, the hexagonal wurtzite structure of ZnO is the most studied crystal. This compound exhibits very interesting and remarkable properties in the field of spintronic, transparent electronics, piezoelectricity and optoelectronics [1,2]. The practical applications of DMS (Diluted Magnetic Semiconductor) in spintronic require that the DMS exhibit ferromagnetism at and above room temperature. On other hand, the discovery of room-temperature ferromagnetism (RT-FM) in transition metal-doped transparent conducting oxides (TCOs) like ZnO or CdO broadens the possibility of application of DMS in modern technology [3,4].

On the other hand, the relationship between hydrogen and magnetic order has recently been found in graphite surfaces by X-ray magnetic circular dichroism [5], important role of this element can be played in the magnetism of non-magnetic materials. Furthermore, hydrogen is one of the most abundant and inevitable impurities, its presence can influence electrical and magnetic properties of ZnO [6].

Recently, some experimental [7–10] and theoretical [11] works have been published concerning the study of the advantageous role of hydrogen to enhancing ferromagnetism formalism in

* Corresponding author.
E-mail address: amina.larani8@gmail.com (A. Larabi).

http://dx.doi.org/10.1016/j.jmmm.2017.09.029
0304-8853/

3d-transition-metal-doped ZnO. It is shown that hydrogen insertion turns out to be a simpler and effective method to generate a magnetic order in ZnO [6,12,13]. In addition, the strong decrease of the electrical resistance provides attractive possibilities for future applications.

It is important to note that among the large number of research papers published so far in the literature, we have mentioned those references particularly, simply because they are directly related to the present work, from which the possible ion valences were used. In the spintronic technological, introducing transition metals like Co, Mn, Fe, Cr, Cu, and Ni has permitted doped ZnO to reveal exceptional magnetic, optical (Room temperature ZnO photoluminescence tuned by Cr doping [14]), and electronic properties required for spintronic materials [15–22]. In this paper, we study the important effect of hydrogen on the electronic and magnetic properties of (Zn, Cr)O. The choice of the Chromium metal transition element is based on the ferromagnetic stability of Cr-doped ZnO DMSs [23,24]. Thus first principles calculations are used to examine the structural, magnetic and electronic properties of Cr-doped ZnO and H-Cr-codoped ZnO. A thorough discussion on the structural properties associated with hydrogen (H) impurities located at several different sites in the lattice is done. Calculations of the total energy allow to identify the most stable position occupied by H in ZnO and (Zn, Cr)O lattice. Similar experimental and theoretical studies have been performed to investigate the behavior of H impurity in Mn doped GaN, Mn doped CdTe and Cr doped ZnO dilute magnetic semiconductor [25–27]. Furthermore, we performed a careful analysis of the Cr-H interactions, and their influence on the structural, electronic and magnetic properties of (Zn, Cr)O.

Table 1
Calculated total energies of the spin polarized state E_{sp}, non-spin polarized state E_{nsp} and absolute total energy differences $|E_{sp} - E_{nsp}|$ by GGA and GGA+U.

	E_{nsp} (eV)	E_{sp} (eV)	$\lvert E_{sp} - E_{nsp}\rvert$ (eV)
GGA	−492.60428	−493.96059	1.356
GGA+U	−489.4936	−491.66209	2.168

2. Computational details

The calculations have been performed using the ab initio total-energy and molecular-dynamics program VASP (Vienna ab intio simulation program) developed at the Fakultät für Physik of the Universität Wien [28,29]. The exchange and correlation energies are treated within the generalized gradient approximation (GGA) [30,31] with projector augmented wave (PAW) [28,32] pseudo-potentials. For the treatment of the semi core *3d* states of Zn and Cr, the generalized gradient approximation with the Hubbard *U* correction method (GGA+U) is used [32,33] with correlation energy correction, $U = 11$ and 3.57 eV for *d* electrons of Zn and Cr atoms, respectively. The exchange parameter *J* has been fixed to 1 eV. The Hubbard *U* value is calculated by varying U in about 0.1 eV steps from 0.0 to 11.2 eV and compared the results of band gap with experimental value. The optimized *U* value showed 2.16 eV for band gap, which is near to experimental value (3.44 eV) [34]. The *U* value obtained in this work differs from that found in other works (9, 10.5, 10.57 and 12.5 eV) [35–38] but it is sufficient to obtain a band gap that matches with that of experiment. The DFT +U approach introduces an on-site correction to better describe

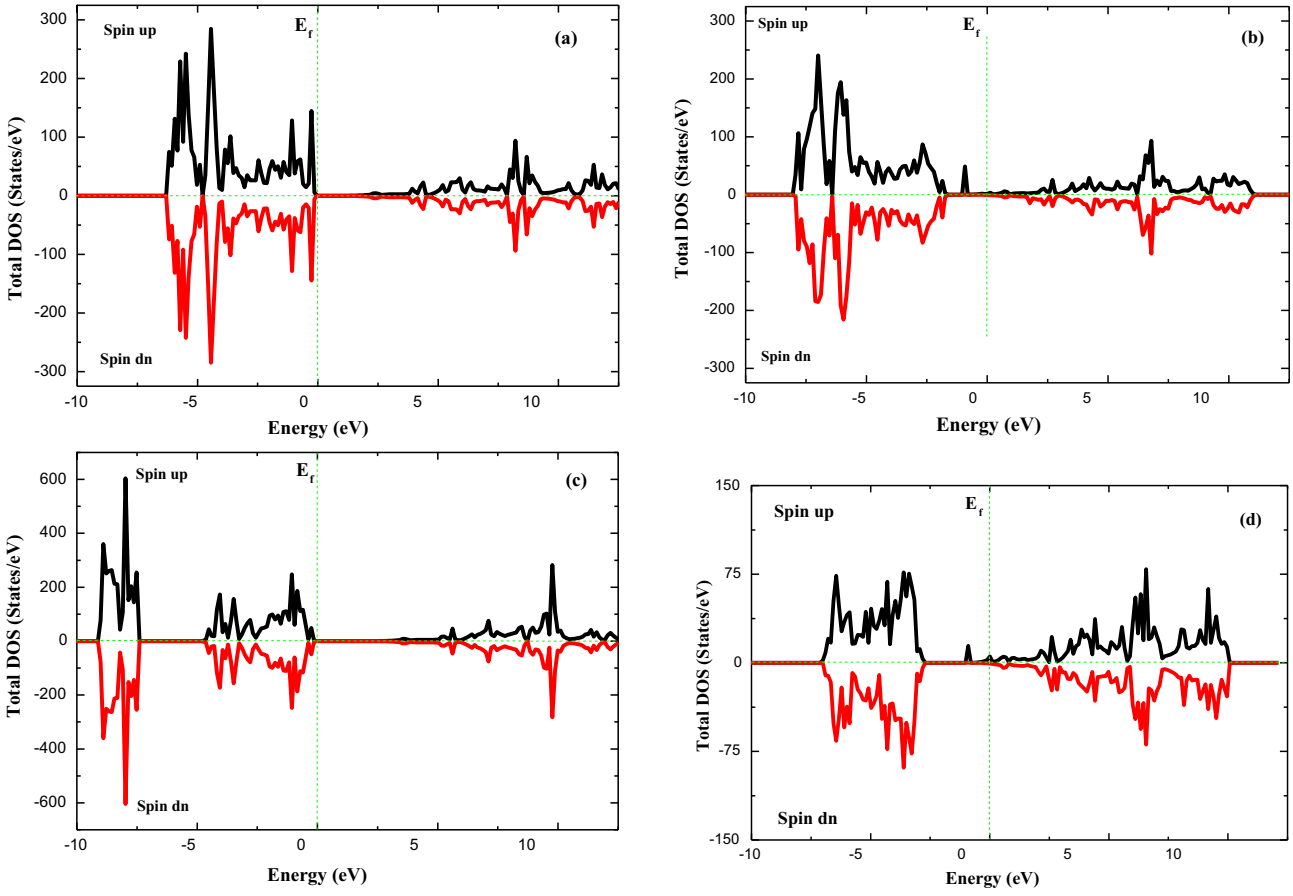

Fig. 1. The total DOS of: pure ZnO ((a) GGA, (c) GGA+U) and a single Cr doped ZnO ((b) GGA, (d) GGA+U).