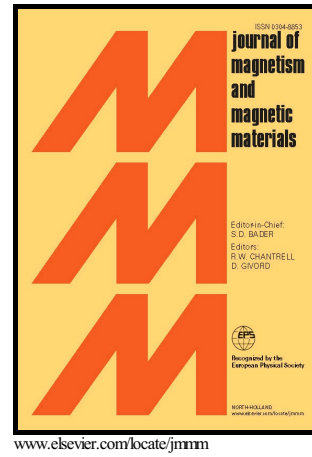


Author's Accepted Manuscript

First principle investigation of structural, electronic and magnetic properties of cubic $\text{Cd}_{0.9375}\text{TM}_{0.0625}\text{S}$ (TM = Ni, Co and Fe)

Hakima Yah, Athmane Meddour



PII: S0304-8853(16)32731-7
DOI: <http://dx.doi.org/10.1016/j.jmmm.2016.12.030>
Reference: MAGMA62238

To appear in: *Journal of Magnetism and Magnetic Materials*

Received date: 23 October 2016
Revised date: 22 November 2016
Accepted date: 4 December 2016

Cite this article as: Hakima Yah and Athmane Meddour, First principle investigation of structural, electronic and magnetic properties of cubic $\text{Cd}_{0.9375}\text{TM}_{0.0625}\text{S}$ (TM = Ni, Co and Fe), *Journal of Magnetism and Magnetic Materials*, <http://dx.doi.org/10.1016/j.jmmm.2016.12.030>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

First principle investigation of structural, electronic and magnetic properties of cubic $\text{Cd}_{0.9375}\text{TM}_{0.0625}\text{S}$ (TM = Ni, Co and Fe)

Hakima Yahia and Athmane Meddour

Author's Affiliations:

Hakima Yahia

Academic degree: Doctor

Laboratoire de Physique des Matériaux, Université 8 Mai 1945 Guelma, BP 401 Guelma 24000, Algérie

Téléphone: +213779506375

E-mail: yahihaki@yahoo.fr

Athmane Meddour

Academic degree: Professor

Laboratoire de Physique des Matériaux, Université 8 Mai 1945 Guelma, BP 401 Guelma 24000, Algérie

Téléphone: +213771959200

E-mail: a_meddour@yahoo.fr

Abstract

In this study, we investigated the structural, electronic and magnetic properties of $\text{Cd}_{0.9375}\text{TM}_{0.0625}\text{S}$ (TM = Ni, Co and Fe) compounds in zinc blende (B3) ferromagnetic phase using all-electron full-potential linear muffin tin orbital (FP-LMTO) calculations within the frame work of the density functional theory and the generalized gradient approximation. The analysis of electronic structures shows that $\text{Cd}_{0.9375}\text{Ni}_{0.0625}\text{S}$, $\text{Cd}_{0.9375}\text{Co}_{0.0625}\text{S}$ and $\text{Cd}_{0.9375}\text{Fe}_{0.0625}\text{S}$ compounds are half-metallic ferromagnets with 100% spin polarization at the Fermi level. This half-metallic behavior is confirmed by the total calculated magnetic moment per Ni, Co and Fe substituted transition metal (TM) atom, which is found to be $2 \mu_B$, $3 \mu_B$ and $4 \mu_B$ for $\text{Cd}_{0.9375}\text{TM}_{0.0625}\text{S}$ (TM = Ni, Co and Fe) compounds, respectively. Furthermore, we found that the TM-3d states are responsible for generating spin-polarization and magnetic moment in these compounds and we establish that the p-d hybridization reduces the local magnetic moment of TM atoms from its free space charge value and produces small local magnetic moments on nonmagnetic Cd and S host sites. Also, we predicted exchange splitting energy $\Delta_x(\text{pd})$ and exchange constants $N_0\alpha$ and $N_0\beta$. The calculated values validate the ferromagnetic nature of these compounds.

Key words

Ab-initio calculations, Diluted magnetic semiconductor, Half-metallic ferromagnetism, Electronic structure, Magnetic properties.

Download English Version:

<https://daneshyari.com/en/article/5491078>

Download Persian Version:

<https://daneshyari.com/article/5491078>

[Daneshyari.com](https://daneshyari.com)