Journal of Alloys and Compounds 737 (2018) 790–797

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

First principles calculations of structural, magnetic and electronic properties of Co_2TiZ (Z = Si and Sn) Heusler alloys using LSDA+U method: Effect of U

M.K. Zayed [a, b], A.A. Elabbar [a, *], O.A. Yassin [a, c]

[a] Department of Physics, Faculty of Science, Taibah University, Madinah, Saudi Arabia
[b] Physics Department, Faculty of Science, Beni-Suief University, Bani-Suief, 6111, Egypt
[c] Department of Physics, Faculty of Science and Technology, Al-Neelain University, Khartoum, 11121, Sudan

ARTICLE INFO

Article history:
Received 1 October 2017
Received in revised form
15 December 2017
Accepted 16 December 2017
Available online 18 December 2017

Keywords:
First principles calculation
LSDA+U
Half metallic
Heusler alloys

ABSTRACT

Using first principles LSDA+U calculation, a systematic investigation of the role of the Hubbard potential *U* on the structural, magnetic and electronic properties of Co_2TiSi and Co_2TiSn Heusler alloys was conducted. The structural, magnetic and electronic properties of Co_2TiSi and Co_2TiSn were calculated at different values of Hubbard potentials for Co (U_{Co}) and *Ti* (U_{Ti}) atoms. The calculated lattice parameters are found to be slightly underestimated when compared with the experimental values with insignificant dependence on both U_{Co} and U_{Ti}. While non integer magnetic moments and metallic behaviors were predicted by LSDA, LSDA+U predicted half metallic behaviors and magnetic moments of $2\mu_B$, in agreement with Slater-Pauling rule, at relatively low values of U_{Co} and U_{Ti}. A strong dependence of the band gap (E_g) on U_{Co} and U_{Ti} was found in the two systems. The $E_g(U)$ dependence is characterized by two distinct regions: first region shows increasing trend while second region shows saturation with the increase in the value of U_{Co}. In the first region, the band gap is controlled by Co d-t_{2g} and Co d-e_g suborbitals only, and U_{Ti} plays no role in agreement with Glanakis et al. scheme. However, in the second region, the band gap is defined by the Co d-t_{2g} and Ti d-e_g suborbitals. The band gaps of the alloys were also calculated using the modified Becke-Johnson (mBJ) method predicting values within the second regions. The role of U_{Co} and U_{Ti} in determining the E_g of the two systems was discussed.

1. Introduction

Half-metallic Heusler alloys have been extensively investigated experimentally and theoretically due to their possible applications in spintronic devices and other technological applications [1]. These materials have majority (spin-up) band that shows a metallic behavior with a nonzero density of states at the Fermi level while the minority (spin-down) band exhibits a semiconducting behavior with a gap at E_F. This 100% spin polarization can be utilized as an ideal current source for spintronic devices. Co-based Heusler alloys Co_2YZ (Y transition metal and Z main group element) are of special interest because they are predicted to be half-metallic ferromagnets (HMF) with a high Curie temperature [1–13].

First-principles calculations using Kohn-Sham density functional theory (DFT) are widely used to investigate electronic structure and magnetic properties of various materials. The success of the DFT in providing vital information on electronic structure is well known. However, DFT suffer from serious drawbacks. One of the major deficiencies of the original Kohn-Sham formulism of the DFT is the underestimation of the band gaps for many materials [14–17]. This band gap problem was addressed and different approximations for the exchange-correlation potentials were proposed. Among these approximations, the local spin density approximation with on-site repulsion parameter (LSDA+U), a method suggested by Anisimov et al. [16] to improve the performance of the DFT, was widely used [17]. The proper value of *U* that would reproduce the materials' properties in LSDA+U calculation is very crucial. Two approaches are commonly used; (i) first-principles based calculations, (ii) treating *U* as an adjustable parameter to reproduce experimentally measured physical properties. In many cases different values of *U*, determined using the first approach, are obtained for the same element, which

* Corresponding author.
E-mail address: elabbar@taibahu.edu.sa (A.A. Elabbar).

https://doi.org/10.1016/j.jallcom.2017.12.166
0925-8388/

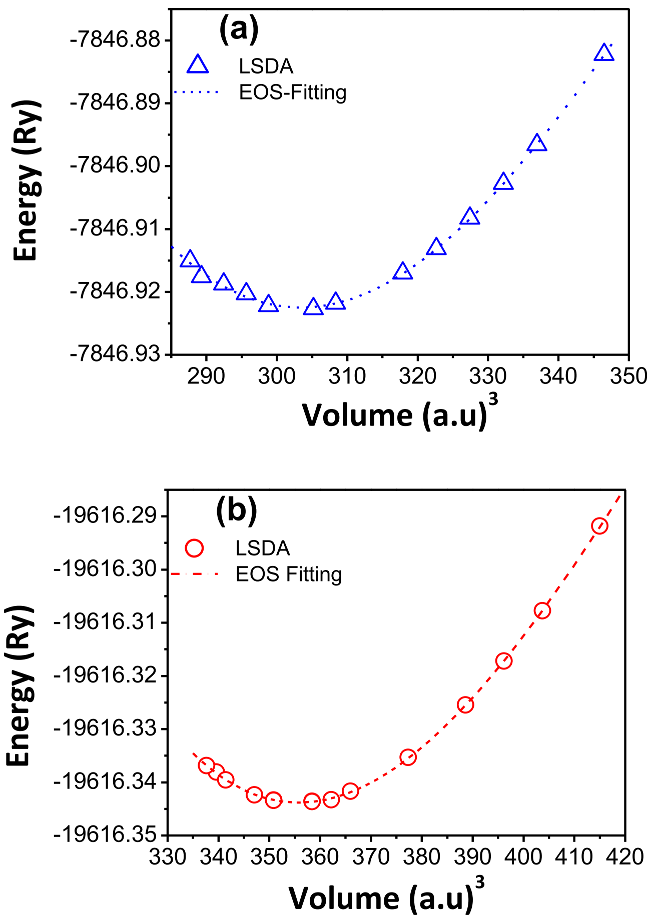

Fig. 1. The total energy of Co_2TiZ systems calculated using LSDA method as a function of the unit cell volume and fitted to the empirical Birch-Murnaghan equation of state (EOS): (a) Co_2TiSi and (b) Co_2TiSn.

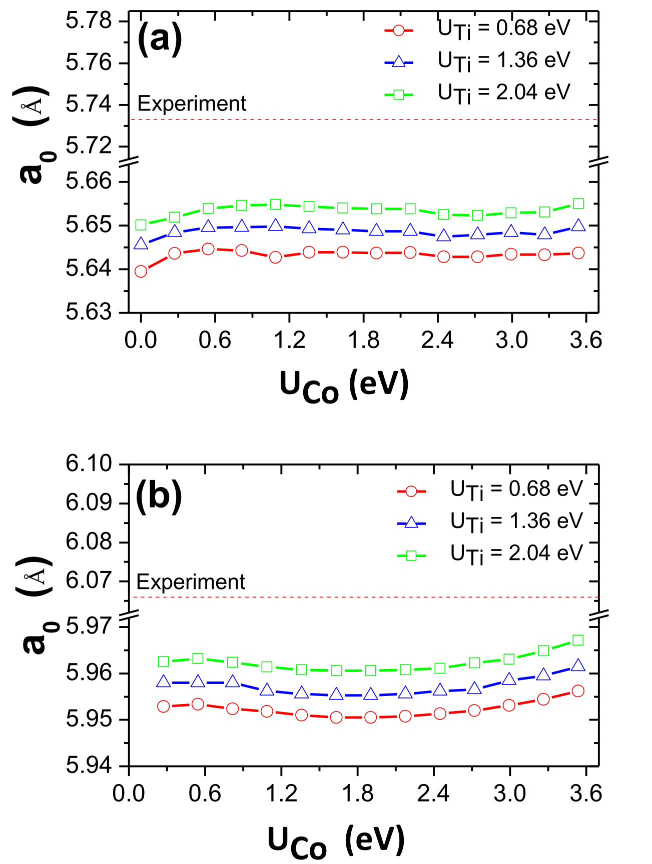

Fig. 2. The calculated LSDA+U equilibrium lattice parameters a_0 with the variation of U_{Co} at different values of U_{Ti} for (a) Co_2TiSi and (b) Co_2TiSn systems.

sometimes is attributed to some technical difficulties in performing calculations [18]. For example, values of U ranging from 2-10 eV were reported for Co 3d orbitals [18–21]. Moreover, the obtained value of U is believed to be dependent on the type of atom as well as the crystal surroundings [17,22]. Therefore, treating U as an adjustable parameter remains a reasonable approach due to the diverse values of U for a given element.

Co_2TiSi and Co_2TiSn are among extensively studied Heusler alloys of promising application in spintronic devices. These alloys are predicted to be half metallic ferromagnets with magnetic moments of 2μ_B in agreement with Slater-Pauling rule [5,6,8–11]. Experimental investigation on these two systems confirmed such predictions and their suitability for thermoelectric and spintronic applications [12,13,23]. To the best of our knowledge, no systematic investigations of the effect of U on structural, magnetic and electronic properties of these two systems have been reported. In the present work, the role of the on-site Hubbard potential on the structural, magnetic and electronic properties are investigated. We have performed first principles calculation for Co_2TiSi and Co_2TiSn Heusler alloys using LSDA+U method. Due to the lack of experimental values of band gap (E_g) in Co_2TiSi and Co_2TiSn, the modified Becke-Johnson (mBJ) [24] method was used to calculate the electronic properties of both systems. This method is reported to be one of the most computationally accessible methods for calculating the band gaps of semiconductors and would be suitable to evaluate the band gap of the half-metallic materials. It is hoped that a detailed analysis of the effect of U on different physical properties of these Heusler alloys can provide an estimate of E_g calculated using reasonable values of U_{Co} and U_{Ti}. A comparison with the results obtained using mBJ method may also provide another support for this estimation.

2. Computational details

The electronic structures have been performed by adopting the full potential linearized augmented plane wave (FP-LAPW) method

Table 1
Some structural, magnetic and electronic properties of Co_2TiSi and Co_2TiSn systems calculated using LSDA, LSDA+U and mBJ.

Co_2TiX	Lattice parameter (Å)		Magnetic moment (μ_B)												E_g (mBJ) (eV)
			LSDA				LSDA+U				mBJ				
	$a_{0(Exp.)}$	$a_{0\ (Calc.)}$	Co	Ti	X	Total	Co	Ti	X	Total	Co	Ti	X	Total	
X = Si	5.740	5.6393	0.783	0.0212	0.0162	1.594	1.180	−0.1723	0.0004	1.9992	1.11003	−0.0630	0.01494	1.99985	1.185
X = Sn	6.072	5.9511	0.8998	0.01874	0.0107	1.804	1.0744	−0.0626	0.00337	2.0004	1.20912	−0.1775	−0.00124	2.00016	1.130