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Original Article

Electronic structure and magnetic properties of Co_2TaAl from ab initio calculations

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ABSTRACT

A first-principles approach is used to study the structural, electronic and magnetic properties of the Co_2TaAl Heusler compound with $CuHg_2Ti$-type structure. The investigation was done using the (FP-LAPW) method where the exchange-correlation potential was calculated with the frame of GGA by Perdew et al. (Phys. Rev. Lett. 77 (1996) 3865). At ambient conditions our calculations predict that Co_2TaAl is half-metallic ferromagnet (HMF) with a magnetic moment of 2 μ_B/fu and HM flip gap of 0.58 eV. In addition, the ferromagnetic phase is found to be energetically more favorable than paramagnetic phase. Therefore, the Co_2TaAl Heusler compound is a candidate material for future spintronic applications.

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1. Introduction

Heusler compounds are ternary intermetallic compounds that have the general composition X_2YZ. In this class, X and Y represent d-electron transition metals, and Z denotes an sp-electron element [1]. In recent years, Heusler compounds have been extensively studied, motivated by their gained importance due to advancements in spintronics [2–6].

Half-metallic ferromagnets (HMFs) meet all the requirements of spintronics, as a result of their exceptional electronic structure. These materials behave like metals with respect to the electrons of one spin direction and like semiconductors with respect to the electrons of the other spin direction. Recently, half-metallic ferromagnetism has been found in, (Ca, Sr, Ba)C [7], Co_2MnSi [8], Co_2MnZ (Z = Ge, Sn) [9], CoFeTiSb [10], Mn_2CoAs [11], ZrFeTiAl, ZrFeTiSi, ZrFeTiGe and ZrNiTiAl [12], $Co_2Mn_{1-x}Fe_xSi$ [13], Co_2MnBi [14] and Co_2FeZ (Z = Al, Ga, Si, Ge) [15].

Generally, Heusler compounds (X_2YZ) crystallize in the cubic $L2_1$ structure (#225), in which the lattice consists of interpenetrating fcc sub lattices with the positions 4a (1/4 1/4 1/4) for the X, 4d (1/2 1/2 1/2) for the Y and 4c (0 0 0) for the Z atoms, respectively. The crystal structures of these compounds are shown in Fig. 1. Our main goal in this work is to evaluate examine the validity of the predictions of half metallicity for Co_2TaAl Heusler compound, the calculations are performed using ab initio full-potential linearized augmented plane wave (FP-LAPW) within the density functional theory DFT within the generalized gradient approximation GGA. Our paper is organized as follows. The theoretical background is presented in Section 2. Results and discussion are presented in Section 3. A summary of the results is given in Section 4.

2. Method of calculations

The first principles calculations were performed by employing FP-LAPW approach [16], based on the DFT [17] as implemented in WIEN2K code [18]. The Kohn–Sham equations are solved self-consistently using FP-LAPW method. In the calculations reported here, we use a parameter $R_{MT}K_{max} = 9$, which determines matrix size (convergence), where K_{max} is the plane wave cut-off and R_{MT} is the smallest of all atomic sphere radii. We have chosen the muffin-tin radii (MT) for Co, Ta and Al to be 2.4, 2.5 and 2.3 (a.u), respectively. The following initial atomic configurations were employed: (Co $3d^7$ $4s^2$), (Ta $5d^3$ $6s^2$) and (Al $3s^2$ $3p^1$). Exchange-correlation effects are treated using GGA as parameterized by Perdew et al. [19]. Self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-6} *Ry*. The convergence criteria for total energy and force are taken as 10^{-5} and 10^{-6} eV/Å, respectively. The valence wave functions inside the

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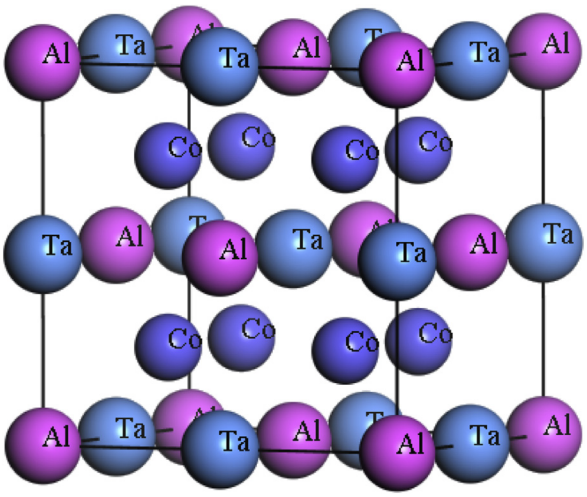

Fig. 1. Crystal structure of Co_2TaAl Heusler compound.

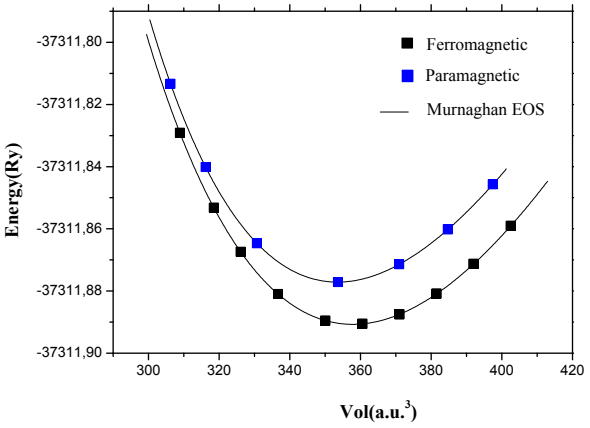

Fig. 2. Volume optimization for the Co_2TaAl Heusler compound.

spheres are expanded up to $l_{max} = 10$ while the charge density was Fourier expanded up to $G_{max} = 14$. The Monkorst-Pack special k-points were performed using 104 special k-points in the irreducible Brillion zone [20].

3. Results and discussion

Our basic procedure in this work is to calculate the total energy as a function of the unit-cell volume around the equilibrium cell volume V_0 for Co_2TaAl Heusler compounds in both paramagnetic and ferromagnetic phases. We present, in Fig. 2, structural optimization curves obtained in both phases, and the data are fitted to the Murnaghan's equation of state [21] so as to determine the ground state properties, such as equilibrium lattice constant a, bulk modulus B and its pressure derivative B'. The calculated structural parameters of Co_2TaAl are reported in Table 1. The optimal lattice parameters obtained by this procedure is in agreement with the experimental value [22]. In the absence of the experimental data regarding the bulk modulus and its pressure derivative B' of the material of interest, and hence our results are predictions. We also include in Table 1 the bulk modulus B and its pressure derivative B' data for Co_2CrAl, Co_2CrGa, Co_2FeAl and Co_2FeGa [23] for comparison purpose. In addition, the ferromagnetic phase is found to be energetically more favorable than paramagnetic phase.

At T = 0 *K*, the calculated spin-polarized band structures of Co_2TaAl compound at the theoretical equilibrium lattice constant along high-symmetry directions of the first Brillouin zone are displayed in Fig. 3. The total and partial densities of states, in which the spin-up and spin-down sub-bands are shown in Fig. 4. The Fermi level set as 0 eV.

In Fig. 3, it is clear that the majority-spin band is metallic, the conduction band minimum (CBM) is found to be mixed with the valence band maximum (VBM) along the (ΓX) direction, while the minority spin band shows a semiconducting gap around the Fermi level. In the minority-spin band, the valence band maximum (VBM) is located at −0.58 eV and the conduction band minimum (CBM) at 0.18 eV. The energy gap for spin-down electrons at around the Fermi level is 0.74 eV and close to the energy gap values for the Co_2MnSi compound [13].

The half-metallic gap [24,25], which is determined as the minimum between the lowest energy of minority (majority) spin conduction bands with respect to the Fermi level and the absolute values of the highest energy of the minority (majority)spin valence bands, is 0.58 eV, for Co_2TaAl compound. This energy gap in the minority-spin band gap leads to 100% spin polarization at the Fermi level, resulting in the half-metallic behavior at equilibrium state. In the absence of both experimental and theoretical data of the energy gap for the material of interest, to the best of our knowledge, no comment can be ascribed to the accuracy of the used method and hence our result may serve only for a reference.

Fig. 4 shows the total density of states and partial density of as a function of energy for the Co_2TaAl compound at its equilibrium lattice constant. To illustrate the nature of the electronic band structures, we have plotted the partial density of states (DOS) of Co e_g and t_{2g}, Ta e_g and t_{2g} and Al-p electrons for the spin-up and spin-down sub-bands. For Co_2TaAl compound, in both spin channels, significant contributions to the total density of states in the energy range between −5.0 and −1.0 eV, come from p electrons of Al element hybridized with e_g electron of Co and t_{2g} states of Ta atom. At the Fermi energy the situation is markedly different, where the t_{2g} orbital of Co and Ta atoms creates fully occupied bands. These values of polarization are similar to those already published for Co_2VZ (Z = Al and Ga) full Heusler compounds calculated with a full-potential linearized augmented plane wave method [26]. In the energy range between 1.0 and 4.0 eV, the e_g were states of Ta atoms contribute to the majority and minority spin states. The origin of

Table 1
Lattice constant a (Å), bulk modulus B (in GPa), pressure derivative of bulk modulus B', total and partial magnetic moment (in μ_B) for Co_2TaAl Heusler compound.

Compound	a	B	B'	m_{Co}	m_{Ta}	m_{Al}	$m_{interstitial}$	m_{Total}
Co_2TaAl(FM)	5.96	205.43	4.94	1.040	−0.008	0.002	−0.075	2.00
Co_2TaAl(PM)	5.93	215.53	5.43	–	–	–	–	–
Co_2TaAl(EX) [22]	5.93	–	–	0.75	–	–	–	1.5
Co_2CrAl [23]	5.70	207.23	–	–	–	−0.038	–	3.00
Co_2CrGa [23]	5.72	208.81	–	–	–	−0.029	–	3.028
Co_2FeAl [23]	5.69	215.87	–	2.74	–	−0.038	–	4.99
Co_2FeGa [23]	5.71	198.85	–	2.76	–	−0.028	–	5.02

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