Spin-polarized DFT Calculation of the Magneto-electronic Properties Under Pressure of the YCrSb Half-heusler Alloy

Ilhem BENAISTI[1], Nacir GUECHI[2], and Mourad DEHBAOUI[3*]

[1]Laboratory of Energy and Smart Systems, Faculty of Science and Technology, University of Khemis Miliana, Algeria

[2]Laboratoire d'Etudes des Surfaces et Interfaces des Matériaux Solides, University Ferhat Abbas Setif 1, Algeria

[3]Laboratoire de Physique des Techniques Expérimentales et ses Applications, Université de Médéa, Algeria

*Corresponding author

Introduction

Half Heusler materials XYZ are typically consisting oftransition metals (X,Y) and an sp-element (Z). These materials are important in spintronics[1]. Half heuslers crystallize in a cubic structure with the space group no.216.

Experimental/Theoretical Study

The spin-polarized electronic structure calculations areperformed using the ultrasoft PP-PW method as applied inthe CASTEP code[3]. The exchange-correlation potential is described using the generalized gradient approximation GGA-PBEsol[4]. The considered valence states are: Y: $4d^1 5s^2$, Cr: $3d^5 4s^1$, Sb: $5s^2 5p^3$. A plane-wave basis set cut-off of 380 eV and a 10×10×10 *k*-points[5] grid for theintegration over the Brillouin zone (BZ) are selected to guarantee sufficiently accurate total energy calculations.

Results and Discussion

A geometry optimization is performed by computing thetotal energy of the unit cell at each fixed pressure for thetype I structure with spin polarized configuration. The calculated total energies versus unit-cell volumes have been fitted to the Birch-Murnaghan equation of states[6] asdisplayed in Fig.1.(a). The calculated equilibrium lattice parameter (a_0) and bulk modulus (B) at zero pressure are 6.3 Å and 72GPa, respectively. These findings agree verywell with those reported in Ref. [2].

As shown in Fig.1.(b) at 0 GPa, the spin-down bands (in red color) have a metallic behaviour with a nonzero density of states at the Fermi level, while, the spin-up bands (in black color) shows a semiconducting nature with an indirect gap Γ-X of 0.93 eV. As a result, YCrSb can be considered as a perfect half-metallic alloy. The variations of valence band maximum VBM and conduction band minimum CBM as functions of pressurefor the spin-up states is shown in Fig.1.(c). One can see that the variation of pressure from -9 GPa to 25GPa do not affect the spin-down bands. Therefore, YCrSb behaves like a metal along this spin channel. Furthermore,from Fig.1. (c), one can also see that VBM is slightly decreases and both CBM and the band gap increase with the increasing of pressure, so we deduce for pressure values less than -3 GPa, YCrSb has a metallic nature, and for pressures range from -3 to 25GPa, YCrSb has a half metallic nature. The calculated total magnetic moment (M_t) of YCrSb is equal to $4\mu_B$ which agree very well with the "M_t=18-Z_t" Slater Pauling rule [1]. For YCrSb, the spin-up bands contain 9electrons and the total number of valence electrons per unit cell (Z_t) is equal to 14. From Fig.1.(d) it is worth to note that the variation of pressuredoes not affect the total magnetic moment of YCrSb.

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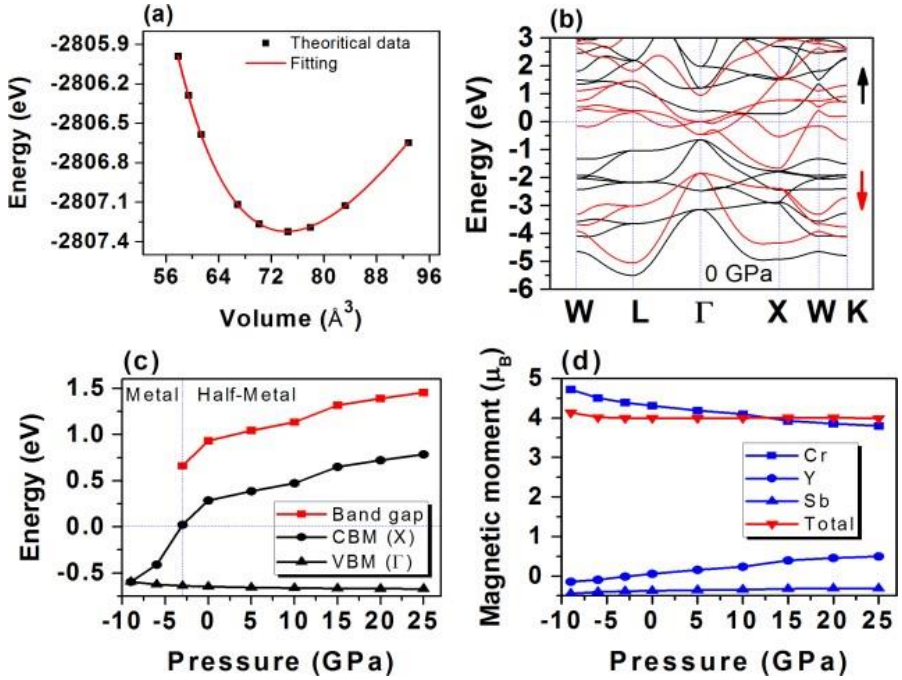

Fig.1. (a) Total energy versus volume per unit cell, **(b)** spin-polarized band structure at 0 GPa, **(c)** pressure effect on the spin-up band gap, and **(d)** pressure effect on the magnetic moments of YCrSb.

Conclusion

In summary, the magneto-electronic properties of the YCrSb Half-Heusler under pressure effect were investigated by using the PP-PW method with the GGA- PBEsol approximation. The calculated band structures indicate that the YCrSb material is a perfect ferromagnetic half metal for a wide range of pressure witha total magnetic moment of 4 μ_B. This value is in good agreement with the "M_t=18-Z_t" Slater-Pauling rule.

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