Structural and Electronic Characteristics of Cubic Half-Heusler Compound AcOF

Shivani Gaur[1,a], Madhu Sarwan[2,b], Sadhna Singh[2,c]

[1] *Department of Physics, Govt. SGS PG. College, Ganjbasoda (M.P.), India.*
[2] *Department of Physics, Barkatullah University, Bhopal (M.P.), India.*

[a] shivanigaur1470@gmail.com
[b] madhusarwan@gmail.com
[c] drsadhna100@gmail.com

Abstract

An investigation has been conducted on structural and electronic characteristics of cubic half heusler compound AcOF. The FP-LAPW approach is used in density functional theory (DFT) to conduct the investigation. GGA scheme was applied to verify the structural stability. The lattice parameter, unit cell volume, bulk modulus, and pressure derivative of bulk modulus are among the ground-state characteristics that are calculated. The calculated GGA lattice parameters correlate well with the available data. Band structure, density of state and charge density have been plotted. Electronic band structure confirms AcOF as an insulator having large Energy band gap.

Keywords: Density functional theory, Structural properties, Electronic properties and Insulator.
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*** Address of correspondence**
Shivani Gaur
Department of Physics, Govt. SGS PG. College Ganjbasoda (M.P.) India.

Email: shivanigaur1470@gmail.com

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Introduction

In general, Half Heusler materials XYZ can be understood as compounds consisting of a covalent and an ionic part. The X and Y atoms have a distinct cat-ionic character, whereas X can be seen as the anionic counterpart. AcOF (XYZ) is ternary inter-metallic half heusler compound consisting Actinium, Oxygen and Fluorine. AcOF crystallizes in the MgAgAs type (FCC) cubic structure with space group F-43m (no. 216), where Ac, O and F atoms are located at 4a(0,0,0), 4b(0.5,0.5,0.5), 4c(0.25,0.25,0.25) Wyckoff positions respectively [1].

Half-Heusler compounds are interesting due to their various properties including semi-conductivity, magnetism, superconductivity, thermoelectricity and half-metallicity [2]. Half-Heusler compounds are also known as topological insulators because of their insulating properties in the interior while metallic nature at the surface [3-4]. Several compounds from this intriguing class of materials, such as LiCdP, LiCdAs, and AgMgAs, have been synthesized. However, only a few have undergone detailed characterization. Beleanu et al. [5] conducted an experimental investigation into the structural and electronic properties of LiMgZ (Z = P, As, and Sb). Their findings suggest that these alloys exhibit semiconducting behavior, with a direct band gap ranging between 1.0 and 2.3 eV. The structural, electronic, thermodynamic properties of Lithium based materials i.e. LiZnP and LiCdP have also been studied [6].

On the other hand, due to band inversion, these materials are found to exhibit topological superconductivity. No studies have been done on the structural, electronic, mechanical and optical properties of AcOF HH compound. In this paper, we have studied its structural and electronic properties and had briefly described the structural properties as well.

Method

In order to understand the physical properties of the compound, density functional theory (DFT) is the most sought and prominent tool to evaluate the compounds, predominately in material science. It is a computational quantum mechanical modelling method used to investigate the electronic structure (or nuclear structure) (principally the ground state) of many body system.

The DFT calculations under the framework of full potential linearized augmented plane wave (FP-LAPW) method available with Wien2k is used to calculate the ground state properties of the compound. The energy exchange correlation effect of energy is studied by the generalized gradient approximation (GGA) scheme. Convergence criteria were set at 0.0001 Ry for energy and 0.0001 elementary charges (e) for charge density, ensuring precise results. The electronic structure was analysed using k-point density of 2000 points to calculate the density of states (DOS). The cut-off value of $RMT*K_{max}$ = 9 (RMT is the smallest muffin-tin radius in the unit cell and K_{max} is the maximum of reciprocal lattice vector) for wave vector is picked that contributes to the plane wave expansion of the wave function in the interstitial region. Inside the atomic sphere, the maximum value of partial waves is l_{max} =10, while in the charge density, the value of G_{max} =12 $(a.u.)^{-1}$. The self-consistent simulations are repeated up to the total energies converged within 10^{-4} Ry.

Result and Discussion

Table 1: Ground state properties of AcOF HH compound.

a (Å)	V (Å) ³	B (GPa)	B’
5.851	338.04	101.84	3.92
5.950 [7]	-	-	-

The half heusler compound AcOF crystallizes in the cubic MgAgAs type structure (space group F-43m No. 216) in which Ac atoms occupy at (0, 0, 0), O atoms at (0.5, 0.5, 0.5) and F atoms at (0.25, 0.25, 0.25) symmetry as shown in Fig. 1. The optimized lattice parameter is 5.851 (Å) as shown in Table 1. In this figure the bond angle between Ac, O and F is represented by light green colour. The bond angle of AcOF is 35.097º and same for AcFO and OAcF i.e. 72.452º for the cubic structure. The bond length of Ac-F is 2.9255 Å and same bond length for the Ac-O and O-F i.e. 4.8514.

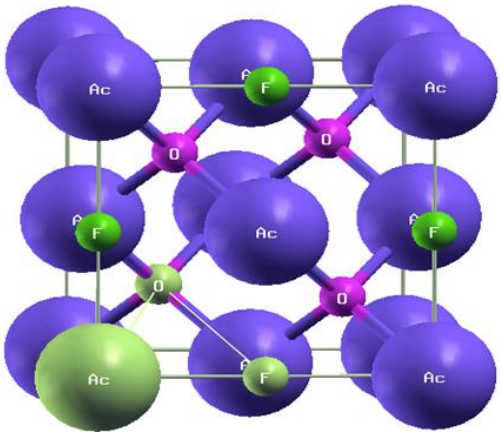

Figure 1: Structure of AcOF

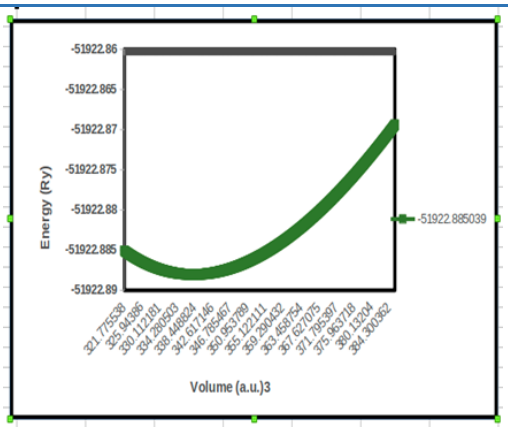

Figure 2: Energy vs volume curve of AcOF.

In Fig. 2, we have plotted energy as a function of volume and the pattern of the curve, which indicates its structural stability at the obtained Volume and Energy parameters. It is also observed from Fig. 2 that GGA calculation provides lowest possible minimum energy indicating a better stability of the compounds. We noticed that this oxide compounds stabilize in the cubic C_{1b} phase with a space group F-43m (216).

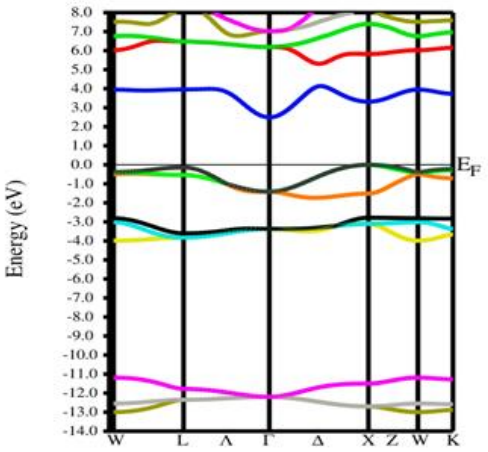

Figure 3: Band Structure of AcOF.

For the calculations of the ground state properties such as the equilibrium lattice constant (a), bulk modulus (B), and its pressure derivative (B’), we have calculated total energy as a function of unit cell volume and befitted to Birch-Murnaghan's equation of state [8] and is displayed in Table 1. The calculated value of lattice parameter is presented in Table 1 together with available theoretical results, which show very good agreement in terms of the ground state properties of the AcOF HH compound.

To achieve a comprehensive understanding of the electronic properties of AcOF a detailed analysis, including band structures and density of states (DOS), has been meticulously presented in next following Figures 3-5. The band structure analysis, shown in Figures-3 along the high-symmetry directions of the Brillouin zone, with the Fermi

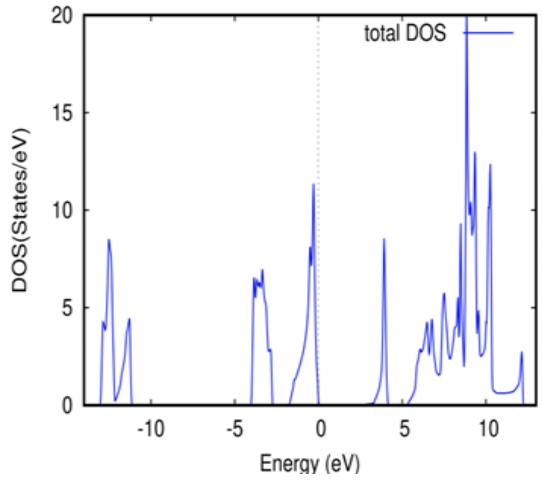

Figure 4: Total density of states (T-Doss) of AcOF.

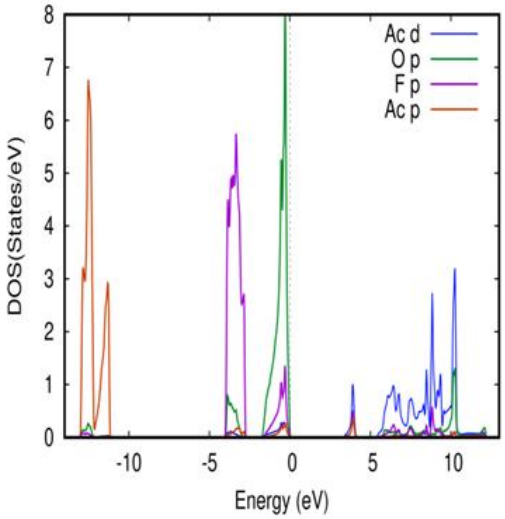

Figure 5: Partial density of states (P-Doss) of AcOF.

level set at 0 eV, confirms the insulator nature of the compound. Band diagram reveal that the lowest energy bands correspond to the Ac-p states, which extend from approximately -13.0 to -11.0 eV, while the F-p states span from approximately -4.0 to -2.9 eV. Further insights into the band structure are offered by the total density of states (TDOS), presented in Figure-4 and the partial density of states (PDOS), illustrated in this Figure-5. A highest peak is observed in O-p state in valence band which dominates near the Fermi level, suggesting an important role in bonding. After this next highest peak is due to Ac-p state showing contributions in the deep valence region (~ -10 eV). F-p state has peaks mainly in the valence band representing the dominant orbital contributions to the electronic states. These figures illustrate the small electronic interactions in AcOF near the Fermi level. A significant hybridization is observed between the O-p, F-p, Ac-p and Ac-d states. No peaks in conduction bands are observed from 0 to 4 eV, highlighting regions of pronounced band gap and density of states.

Conclusion

The structural and electronic properties of AcOF have been investigated by using FP-LAPW method within GGA. The structural stability is confirmed by the energy versus volume curve and found that it is dynamically stable in fcc cubic MgAgAs-type structure. The computed values of lattice parameters are impressively matched with other available data, though the rest of the ground-state properties are never reported before. From electronic analysis, it is seen that AcOF as a topological insulator having large band gap. In the valence band p state of O (oxygen) is near the Fermi level confirming the topological behaviour. After that large band gap is observed between valance and conduction band.

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