Computational Study of Rare Earth Intermetallic

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Abstract.

First-principle calculations are quantum mechanical computing techniques that frequently use density functional theory (DFT) to comprehensively examine the structural and electrical characteristics of a binary rare earth intermetallic complex. Through the solution of equations pertaining to a system's electrical structure, these techniques enable extremely precise predictions of material properties. Under normal circumstances, the intermetallic compound under study shows stability in a CsCl-type B2 structure. This structural type describes a basic cubic crystal structure in which the centre of the cube is occupied by one type of atom (such as Hg) and the corners by another type (such as Ce). Many binary intermetallics have this configuration, which is linked to particular symmetry and bonding characteristics. Parameters like the bulk modulus, which measures the material's resistance to compression, the lattice constant, which measures the length of the unit cell edge, and the pressure derivative of the bulk modulus, which shows how the bulk modulus varies with applied pressure, are calculated in order to comprehend the mechanical properties of this compound. When evaluating the material's mechanical stability and behaviour under various pressure settings, these criteria are essential. The band structure and density of states (DOS) of the compound CeHg are examined from an electronic point of view.

The DOS shows how many electronic states are possible at each energy level, whereas the band structure shows how the electrons' energy levels are spread over various momentum states. According to the research, CeHg does not have a band gap, meaning that there is no energy range between the conduction band (unoccupied states) and the valence band (occupied states) where no electronic states exist. CeHg is categorized as a metal rather than a semiconductor or insulator due to the lack of a band gap. These results show that

CeHg has metallic behaviour, which means that its free electrons allow it to conduct electricity effectively. Because of these characteristics, it could be used in applications where metallic conductivity is crucial.

KEY WORDS: Computational Study, Phase Transition, Rare Earth Intermetallic

1. INTRODUCTION

Intermetallic compounds are materials that consist of two or more metallic elements bonded together in a specific stoichiometric ratio, often forming a distinct crystal structure. These compounds are distinguished by a combination of remarkable physical and chemical properties that make them attractive for advanced applications. One key feature of intermetallic compounds is their high specific strength, which refers to their strength-to-weight ratio. This means they are exceptionally strong for their mass, making them particularly valuable in applications where weight is a critical factor, such as aerospace and automotive industries. Additionally, these materials possess a high melting point, enabling them to retain their structural integrity and performance under extreme thermal conditions.

Despite these advantages, intermetallic compounds are often brittle in nature. This brittleness arises from their strong internal order and mixed bonding character, which limits their ability to deform plastically under stress. As a result, while they are excellent for static and high-temperature structural applications, their fragility can present challenges in dynamic or impact-loading scenarios. Their combination of properties makes intermetallics potential candidates for high-temperature structural materials, especially in aerospace applications, where materials must withstand high mechanical loads and extreme temperatures without significant degradation. Beyond structural uses, intermetallic compounds also exhibit good

electrical and magnetic properties, which can be leveraged in electronic and magnetic devices. Intermetallic compounds often serve as a bridge between metallic and ceramic properties. Metals are known for their ductility, electrical conductivity, and toughness, while ceramics are appreciated for their hardness, high melting points, and chemical stability. Intermetallics combine aspects of both, offering a balance of mechanical strength, thermal stability, and unique electronic or magnetic characteristics. The bonding in intermetallics is typically a mixture of metallic, covalent, and ionic types. This mixed bonding contributes to their strong internal order (a highly organized atomic arrangement) and underpins many of their desirable traits, such as their ability to exhibit chemical resistance, magnetic behavior, and even superconducting properties in certain cases. These properties make intermetallic compounds valuable in diverse applications, ranging from turbine blades and heat-resistant coatings to advanced electronics and magnetic materials [1,2].

Among the group of intermetallic compounds CeHg belongs to rare earth intermetallics. Indelli et al. concluded that the present compound has CsCl type structure using X-ray study [3]. Spin polarized ab initio calculations have been carried out to study the structural, electronic, elastic and thermal properties of CeHg intermetallic compound in B2 structure by Devi et al. [4]. CeHg is less explored intermetallic in the group of rare earth intermetallic compounds. In summary, intermetallic compounds are advanced materials that combine high mechanical performance with appealing electrical, magnetic, and thermal properties. Their ability to operate effectively in extreme conditions and their unique balance of metallic and ceramic characteristics make them a focus of research and development for high-tech applications.

In this study structural and electronic properties of CeHg have been reported. DFT functional hybrid PBE has been used to perform this investigation. The ground state properties of present compound have been calculated. Moreover, this paper also has been stimulatedthe electronic band structure (BS) and density of states (DOS) for the present compounds.The method of computation is described in Section 2.In Section 3, results with some performedusing the first principles pseudopotentialpredictions are discussed.

2. METHODS OF CALCULATION

Quantum espresso is a computational technique for first principle calculation of periodic as well as disordered systems. It is mainly based on DFT theory (electron-ion interaction), plane wave and pseudopotentials (electron-electron interaction). It calculates the ground state energy and Kohn Sham orbital for both insulators and metals and various types of structural optimizations. Quantum espresso can be used to study metals, semiconductors as well as insulators. Three main components of method are PWSCF (Plane wave self consistent field), CP (Car Parinello), FPMD (First principle molecular dynamics). For quantum espresso irreducible k-points are generated according to the Monkhorst-Pack scheme [5]. The Kohn-Sham single-particle functions were expanded on a basis of plane-wave set with a kinetic energy cut-off of 34 Ry. Brilliouin-zone was sampled with 12x12x12 k-point mesh, in order to get well converged ground state energy. The exchange and correlation effects have been treated within the GGA. The lattice parameter, bulk modulus and pressure derivative of the bulk modulus were determined by the standard procedure of computing the total energy for different volumes and fitted to Murnaghan's equation of state [6]. (PWSCF) method. The equilibrium lattice constants were obtained by minimizing the total energy. These parameters were used in the non self-consistent calculations for band structure. These energy values have been fitted to the Murnaghan's equation of state [6]

to obtain the equilibrium lattice constant (a), bulk modulus (B) and its pressure derivative (B′) at minimum equilibrium volume V0

$$P(V) = \frac{B}{B'}\left[\left(\frac{V_0}{V}\right)^{B'} - 1\right] \quad (1)$$

Where the fit parameter are the equilibrium volume V0, the bulk modulus B:

$$B = -V\frac{\partial P}{\partial V} = V\frac{\partial^2 E}{\partial V^2} \quad (2)$$

And its derivative with respect to the pressure, B’ = dB/dP. In Table-1 the calculated structural parameters are tabulated. These parameters are compared with available results. It is clearly indicate that our results are in good agreement with the available experimental [3] and other theoretical results [4].

3. RESULT AND DISCUSSION

Fundamental characteristics of a material that measure its resistance to deformation under mechanical stress are called elastic constants. These constants are crucial for comprehending the material's response to forces in a variety of applications and offer insights into the material's stability and mechanical behaviour. There are just three separate elastic constants for a material having a cubic crystal structure, C_{11} explains the ability to withstand longitudinal deformation along the primary crystallographic axes, such as compressed or stretched along one axis. C_{12} shows how deformation in one direction influences another by linking strains along two perpendicular axes. C_{44} concerns the material's ability to withstand sliding planes within the

crystal structure, or shear deformation. These three constants are sufficient to fully describe the elastic behaviour of a cubic system due to its high degree of symmetry.

A material must have a positive strain energy under any arbitrary deformation in order to be considered mechanically stable. This criterion places particular restrictions on a cubic material's elastic constants. Assures that the material does not stretch or compress along the primary axes ($C_{11}>C_{12}$, $C_{44} > 0$ and $C_{11}+2C_{12}>0$). The materials' mechanical stability is confirmed by the elastic constants computed for them, which meet these stability requirements.

Density functional theory (DFT) makes extensive use of the Generalized Gradient Approximation (GGA) framework, which includes the PWSCF (Plane-Wave Self-Consistent Field) approach. This technique works especially well for making highly accurate predictions about the mechanical and electrical characteristics of crystalline materials. Table 1 displays the outcomes for every calculated parameter, including derived mechanical characteristics and elastic constants. Additionally, there is good consistency between the published numbers and earlier computations or experimental results, if available. This validation demonstrates the material's potential for a range of applications and reinforces the computations' dependability.

Table-1 Ground State properties of CeHg.

Solid	Approach	a (Å)	B	B'	C_{11}	C_{12}	C_{44}	B/G
CeHg	Present							
	Others Theoretical	3.821[a]	57.41[a]	3.49[a]	122.81[a]	28.54[a]	42.86[a]	1.34[a]
	Others Theoretical	3.702[a]	68.89[a]	4.21[a]	125.03[a]	31.23[a]	34.04[a]	-
	Experimental	3.816[a]	-		-	-	-	-

a- ref [4]

Elastic constants are the basic material parameters that describe the resistance of the material against applied mechanical deformation. We know that there are only three independent elastic constants namely C_{11}, C_{12} and C_{44} in cubic system [6]. The criteria for mechanical stability of any compound is that the strain energy should be positive, which imposes further restriction on the values of the elastic constants [7] such as$C_{11}>C_{12}$; $C_{44}>0$; $C_{11}+2C_{12}>0$. For mechanical stability these criteria are satisfied by the calculated elastic constants of all the compounds under study. Our reported values of elastic constants C_{11}, C_{12} and C_{44} satisfy these criteria and are reported in Table-1.

In addition for exploring the electronic properties the electronic band structure (BS), total density of states (TDOS) and partial density of states (PDOS) of CeHg are studied. These electronic properties are presented in Fig. 1, 2 and 3 respectively. To find the equilibrium atomic structure of the crystal the minimization of total energy is calculated.

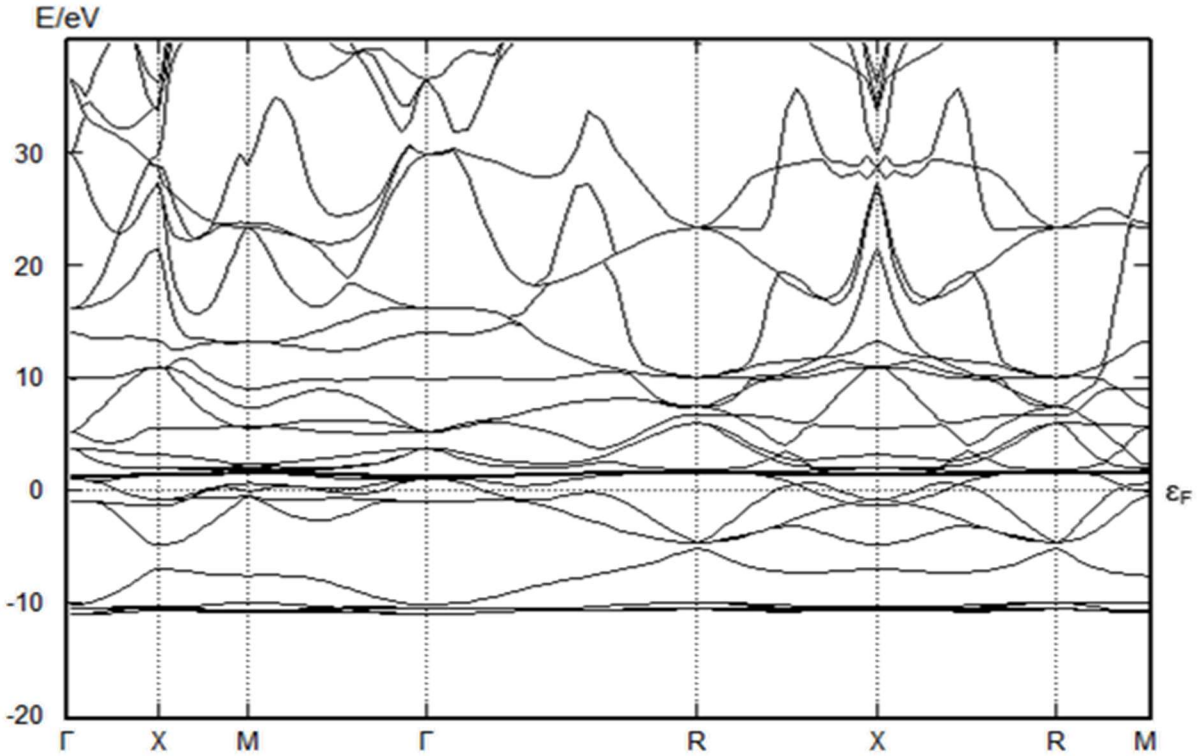

Fig: 1 Electronic band structure of CeHg in CsCl-Phase

The electronic band structure calculations presented in Fig. 1. This figure shows that CeHg exhibit metallic character. The analysis of TDOS is presented in Fig. 2 and also revealed that Fermi energy is mainly composed of 4fstates of rare earth element. Further the PDOS of CeHg in CsCl phase are presented in Fig. 3. The s, p, d and f states of present intermetallic are analysed through this figure**.**

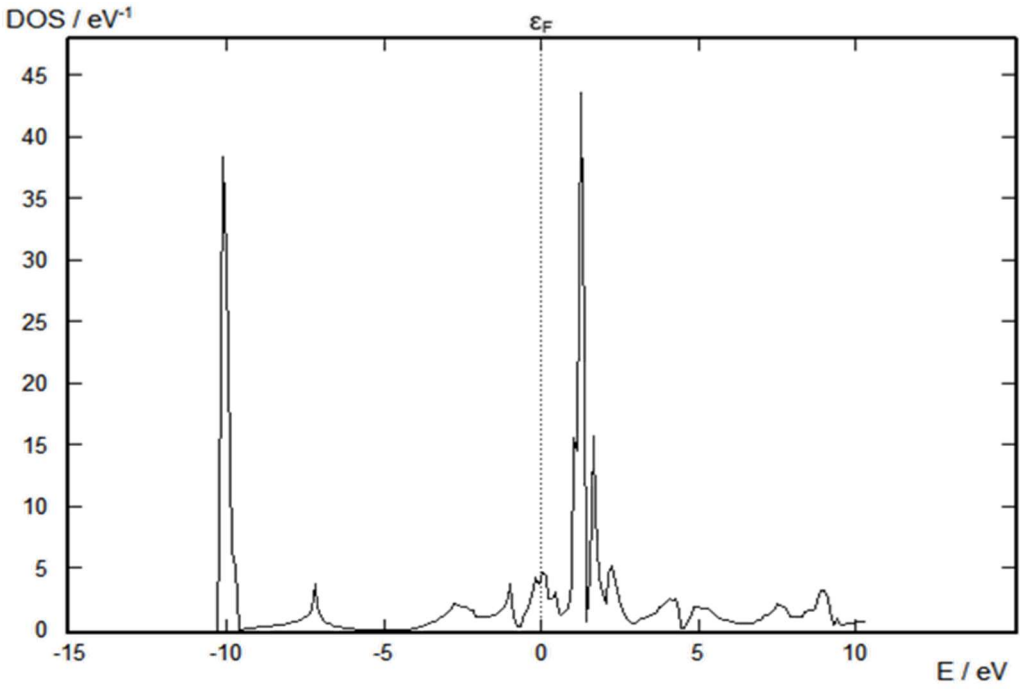

Fig: 2 Density of state (DOS)of CeHg in CsCl-phase.

The electronic band structure calculations for CeHg are presented in Fig. 1, providing a graphical representation of the energy levels of electrons within the material as a function of their momentum. This is a fundamental tool for understanding the electronic properties of materials.

The band structure reveals that CeHg exhibits metallic character, meaning that there is no energy gap (band gap) between the valence band (occupied states) and the conduction band (unoccupied states). Instead, the bands overlap at the Fermi energy level, which is the highest occupied energy level at absolute zero temperature. This overlap allows free electrons to move easily, confirming the material's ability to conduct electricity efficiently.

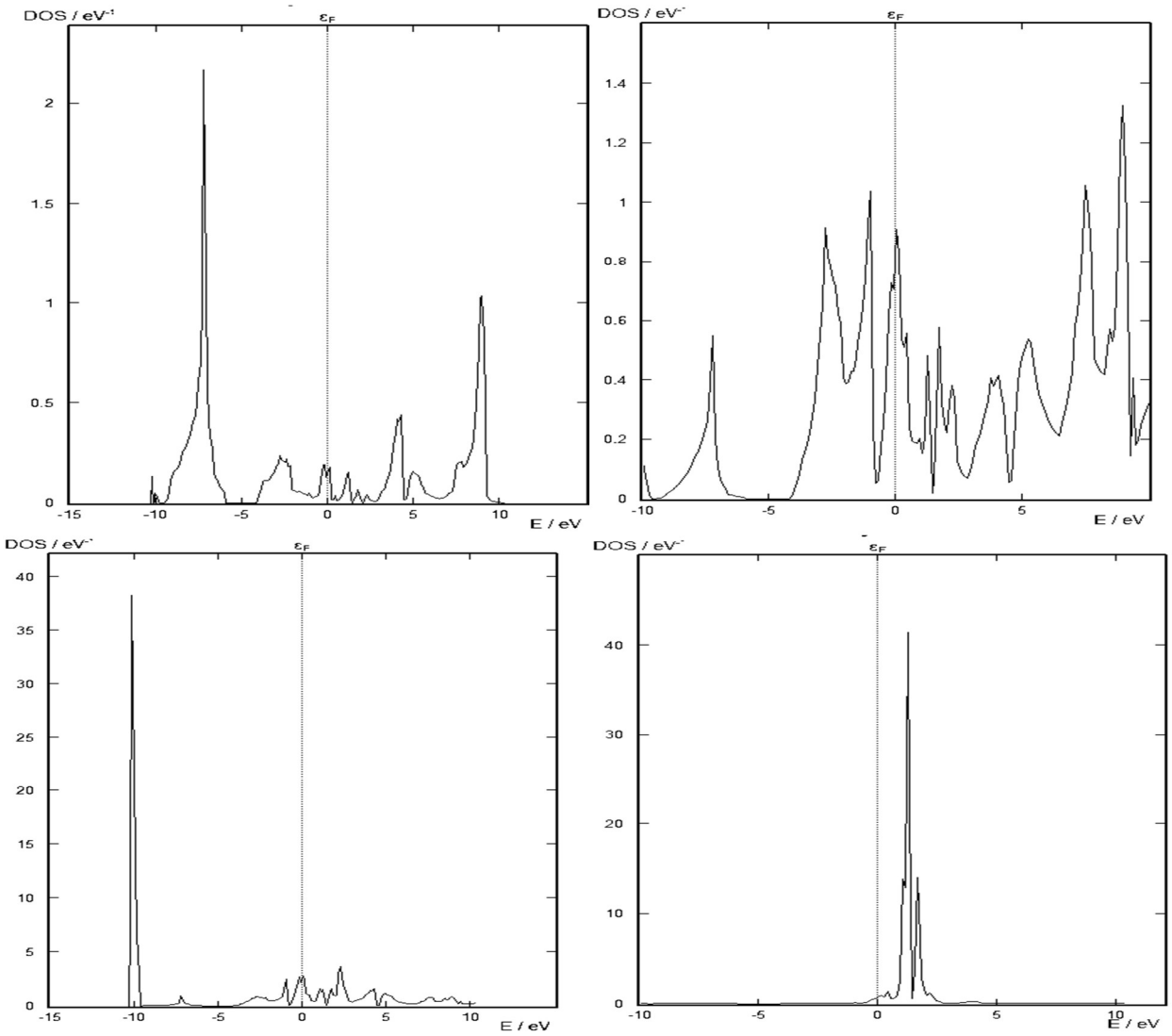

Fig: 3
Partial density of state (PDOS) of CeHg in CsCl-phase.

The Total Density of States (TDOS) for CeHg is presented in Fig. 2, providing a quantitative view of the number of electronic states available at each energy level. From the TDOS analysis, it is observed that the Fermi energy (the energy level at which electronic states are occupied at absolute zero) is primarily composed of the 4f states of the rare earth element Ce. This indicates that the electronic properties and metallic behavior of CeHg are strongly influenced by the contribution of these localized 4f orbitals, which are characteristic of rare earth elements. These 4f states typically lie close to the Fermi level and can have a significant impact on the material's electronic, magnetic, and optical properties.

4. CONCLUSION

CeHg's metallic nature indicates that it is appropriate for uses where high electrical conductivity is necessary. The significance of Ce's electronic structure in influencing the behaviour of the material is highlighted by the predominance of 4f states close to the Fermi energy. Understanding how the atomic orbitals of Ce and Hg contribute to the overall electronic structure is made possible by the thorough PDOS analysis. This information can be used to customize the material's characteristics for particular uses, such as in electronics, catalysis, or magnetic materials.

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