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Ab-initio calculations of Structural and Electronic Properties of REHg (RE = Ho and Er) intermetallic compounds

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ABSTRACT: Spin polarized ab-initio calculations have been carried out to study the structural and electronic properties of REHg (RE = Ho and Er) intermetallic compounds in B_2 crystal structure. The calculations have been performed by using both generalized gradient approximation (GGA) and local spin density approximation (LSDA). The calculated values of lattice constant (a_0) for these compounds with GGA and LSDA, are in good agreement with the experimental data. The bulk Modulus (B), first order derivative of bulk modulus (B') and magnetic moment (μ_B) are also calculated. The band structure and density of states are plotted which reveal the metallic nature for both compounds.The energy band structure and electron density of states show the occupancy of 4f states.

Keywords: Ab- initio Calculation, Electronic properties, Band structure, Magnetic moment.

I. INTRODUCTION

The intermetallic compounds with B_2-type structure have intensely attracted considerable attention, due to their physical and mechanical properties that are often superior to ordinary metals, such as high strength, melting at high temperature, low specific weight, and good corrosion resistance [1, 2]. Intermetallic compounds are among the most important solid state materials because of their diverse physical properties and widespread use in numerous applications. These intermetallics can be denoted as the chemical formula RM, where R indicates

a rare-earth element, and M indicates a late transition metal or an early p-element. However, most intermetallic alloys exhibit brittle behavior at room temperature, which limits their engineering applications, in both single crystal and polycrystalline states. In 2003, a new class of high ordered, ductile intermetallic compounds with B_2 structure was discovered by Gschneidner et al. [3]. A well-known property of the rare earth elements is their incomplete 4f shell, which becomes progressively filled in going from La to Lu. The shielding of the 4f shell leads to interesting physical properties which differ from one lanthanide ion to the next by the number of electrons compacted in the 4f shell. Rare earth based intermetallics REHg (RE = Ho and Er) are binary intermetallic compounds with CsCl structure, which belong to Pm3m space group (no 221). Indelli *et al.* [4] have predicted that these compounds are stable in B_2 phase and calculated the lattice parameters at ambient conditions by using X-ray diffraction technique. Apart from the experimental lattice parameter of these intermetallics no systematic experimental or theoretical results on the structural and electronic properties are available in literature. In the present paper a comprehensive and systematic study related to the structural and electronic, properties for these compounds has been carried out.

II. METHOD OF CALCULATION

REHg (RE= Ho and Er) compound crystallizes in a simple cubic B_2 structure with four atoms per unit cell. It belongs to the *Pm3m* space group with RE atoms occupying the corners of the cube while the Hg atoms occupying the cube faces. First-principles study of the REHg compound was performed by employing full potential linearized augmented plane wave (FP-LAPW) method [5] based on density functional theory within the generalized gradient approximation (GGA) incorporated in the WIEN2k code [6]. It is a variational method that is at present the most successful approach to compute the electronic structure of matter. The density functional theory is derived from the N- particle Schrodinger equation and useful for system of many electrons.

The exchange correlation potential is treated with generalized gradient approximations in the scheme of Perdew, Burke and Ernzhof (PBE-GGA) [7], Wu and Cohen (WC-GGA) [8] and Perdew *et al.* (PBEsol-GGA) [9] to investigate the structural and electronic properties of REHg compounds. The basis function has been expanded up to Rmt x K_{max} = 7.0, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is l_{max} = 10 while the charge density is Fourier expanded up to G_{max} = 12. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [10] to obtain the ground state properties. The energy band structure and corresponding density of states are prominent quantities that determine the electronic structure of a system. The non spin polarized calculation has been performed using LSDA approximation to understand the electronic behavior of REHg intermetallic compound in terms of electronic band structure (BS) and density of states (DOS). Also, it is one among the most accurate scheme for band structure calculations. It is based on full-potential (linearized) augmented plane-wave ((L) APW) + local orbitals (lo) method, one of the most accurate schemes for band structure calculations. We have used an optimized geometry obtained through a self consistent process to investigate the electronic structure of the crystal lattice of the material.

III. RESULT AND DISCUSSION

A. Structural Properties

In order to calculate the ground state properties of mercury based intermetallic REHg (RE = Ho and Er), the total energies are calculated as a function of reduced volume in B_2-type (CsCl) structure using full potential linearized augmented plane wave (FP-LAPW) method. The equilibrium lattice constant can be obtained by fitting the total energy vs. optimized volume data fitted to the Birch-Murnaghan equation of state. All the results are listed in table 1. REHg compounds are found to be stable in B_2- phase at ambient pressure. An inspection of table 1, reveals that the bulk modulus of ErHg is higher than that of HoHg, indicating that ErHg is harder than HoHg. As shown in table 1, the calculated lattice constants for both the compounds are compared with the available experimental data [5]. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its first derivative (B') for REHg have been calculated in their B_2-phase by all the GGA approximations mentioned. We have also found the values of magnetic moment (μ_B) of REHg and presented it in table 1. It is revealed from table 1 that the calculated values of equilibrium lattice constants a_0 are in reasonable agreement with the available experimental data.

Table 1 : The calculated structural and electronic properties of REHg(RE= Ho and Er).

Solid	Approx.	a_0 (Å)	B (GPa)	B′ (GPA)	μ_B	$N(E_f)$ (states/eV)
HoHg	PBE-GGA	3.7428	51.54	4.50	3.50	0.55↑
	WC-GGA	3.6630	59.02	4.53		14.09↓
	LSDA	3.6009	70.17	4.44		
	PBESol-GGA	3.6559	59.81	4.78		
	Exp.	3.660[a]	-	-		
ErHg	PBE-GGA	3.7219	56.55	5.32	2.49	0.53↑
	WC-GGA	3.6532	66.32	5.45		5.74↓
	LSDA	3.6025	76.16	5.28		
	PBESol-GGA	3.6512	70.04	3.26		
	Exp.	3.645[a]				

[a]Ref[5]

B. Electronic Properties

The electronic energy band structures along the principal symmetry directions for REHg in B_2 phase are presented in Fig1 (a) and (b). The band structures are calculated along the path that contains the highest symmetry points in the Brillouin zone, namely $R \rightarrow \Lambda \rightarrow \Gamma \rightarrow \Delta \rightarrow X \rightarrow Z \rightarrow M \rightarrow \Sigma \rightarrow \Gamma$.

The energy zero is set at the Fermi level. The lowest lying band in both REHg compounds resulting mainly from ‘5*d* ’ state of Hg. The difference in the spin up and spin down bands is primarily due to the ‘4*f* ’ states.

The occupied spin up ‘4*f* ’ states are below the E_f and around -2.0 eV while the spin down 4f states stages gets shifted at the E_f around 0.1 to 0.2 eV for both REHg.

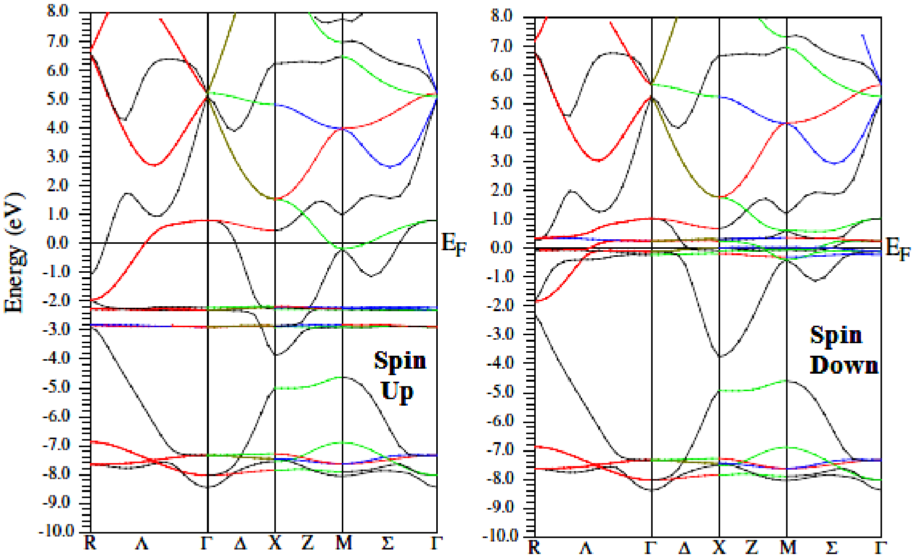

Fig1 (a) Band Structure of HoHg

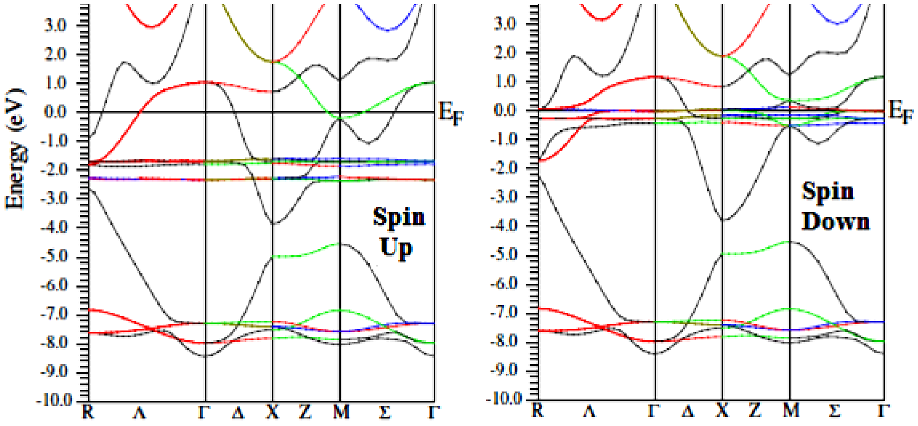

Fig1 (b) Band Structure of ErHg

To further reveal the nature of the electronic band structures and the bonding situation, we have also calculated the total and partial density of states (DOS) for REHg is presented in Fig 2(a) and (b). At the Fermi level, the density of states for these compounds are greater than 0, hence exhibit in saz metallic behavior. The ‘4*f* ’ states are easily identified as sharp peaks in the total DOS. Generally, the ‘4*f* ’ states are highly localized and lie at or close to E_f in REHg compounds for spin up channel while these states are gets shifted towards the conduction region for spin down channel. The conduction band mainly consists of ‘*d* ’ state of Hg atoms. The delocalized ‘4*f* ’ states of RE are situated around -3.0 eV to -1.0 eV in valence region in spin up mode whereas around -1.0 eV to 0.5 ev in spin down mode. The metallicity is observed due to ‘4*f* ’ states of both RE and Hg with little contribution of ‘5*d*’ state of Hg atoms. The finite values of DOS at the Fermi level for both REHg compounds are listed in table 1.

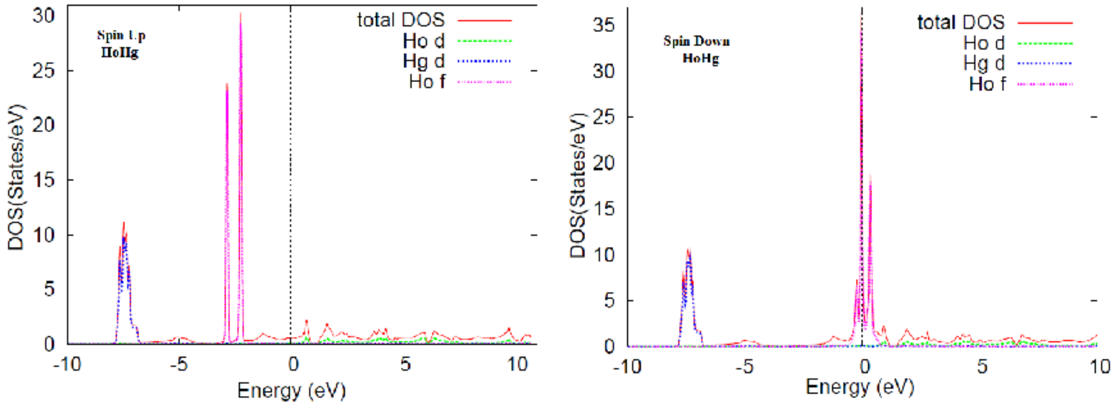

Fig. 1(a)

The Density of States of HoHg.

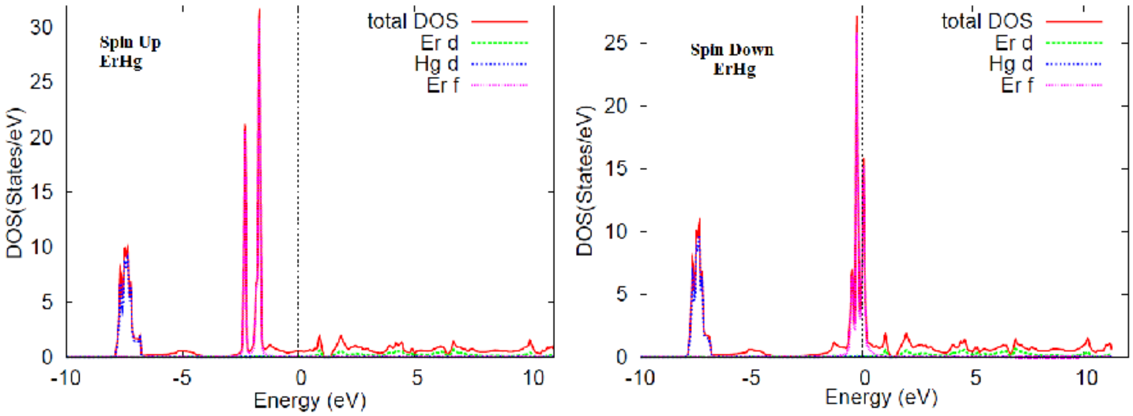

Fig. 2(b) The Density of States of ErHg.

IV. CONCLUSION

In this work, We have investigated the structural and electronic properties of REHg (RE = Ho and Er) compounds. We have systematically studied these compounds by using the FP-LAPW method based on density functional theory, within different Schemes of approximations, PBE-GGA, WC-GGA, PBEsol-GGA and LSDA as the exchange correlation potential. The electronic properties of these compounds are studied by calculating band structures and its corresponding density of states. The electronic band structure calculation shows that all the studied compounds have zero band gap values and show metallic nature.

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