

Study of Structural and Electronic Properties of CeZn₂

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ABSTRACT

The full-potential linear augmented plane wave plus local orbital (FP-LAPW+lo) method employing the generalized gradient approximation (GGA) has been used to study the structural and electronic properties of CeZn₂. The structural properties have been studied in terms of energy vs. volume curve histogram and some parameters viz. lattice constants (a), bulk modulus (B_0) and its pressure derivative (B_0') whereas electronic behavior has been represented in terms of total valance charge density distribution, band structure and density of states histograms. The electronic study indicate that “s” and “d” orbital electrons of Zn have dominant character below the Fermi level, while Ce-f empty states are existed above the Fermi level for the conduction.

Keywords: Rare Earth Intermetallics Structural Properties, Electronic Structure.

I. INTRODUCTION

The prototype rare earth intermetallic compound, CeZn₂ is crystallized in the orthorhombic phase (74-Imma) [1]. It shows unexpected physical behavior due to localization of 4f-electrons (position of 4f-density of states with respect to Fermi level). The positions of 4f-density of states demonstrate the degree of hybridization between localized 4f and conduction bands. There are large number of binary rare earth intermetallic compounds like (REX, RE= rare earth elements and X = Cu, Zn, Cd, Ag etc) which are used as high temperature structural materials for automobile and aerospace applications due to their high ductility [2-6]. It may be interesting to study the structural and electronic properties of these compounds by modifying the ratio of RE and X. Thus, CeZn₂ have been chosen with this idea for the study which may be better alternative of binary rare earth intermetallics. To best of our knowledge, many workers have made the study on many other REX₂ (RE = rare earth elements, X = transition element) proto type compounds [7-11], but the studies of structural and electronic properties of CeZn₂ compound have not been made which are important properties to search the new materials for future applications. Thus, CeZn₂ have been chosen for the study. In the present study, we have performed first principle calculations to study structural behavior in terms of energy vs. volume curve histogram and some parameters viz. lattice parameters, bulk modulus and its first order pressure derivative along

with electronic behavior in terms of total valance charge density distribution, density of states and band structure histograms.

II. COMPUTATIONAL METHOD

In the present study, the calculations have been made on density functional theory (DFT) implemented in WIEN2k package [12-14] to investigate the structural and electronic properties of CeZn₂. The advanced method of full-potential (linear) augmented plane wave plus local orbital (FP-APW+ lo) [12] has been used to linearize the energies which is highly accurate technique based on DFT. For structural and electronic properties, we have used generalized gradient approximation (GGA) [15] for calculating the exchange and correlation energy. In GGA approximation, the basis set is obtained by dividing the unit cell into non-overlapping atomic spheres and an interstitial region. Inside the atomic sphere a linear combination of radial function times the spherical harmonics is used; in the interstitial region, a plane wave expansion is augmented by an atomic like function in each atomic sphere. The k and E convergence are checked by increasing the number of k points and the energy convergence criteria. In the irreducible part of the Brillouin zone, 10 x 10 x 10 k points were used to calculate the total and partial density of states.

III. RESULTS AND DISCUSSION

3.1 Structural properties

The prototype rare earth intermetallic compound CeZn₂, is found to be stable in the orthorhombic phase with lattice parameters ($a = 4.635 \text{ \AA}$, $b = 7.540 \text{ \AA}$, $c = 7.501 \text{ \AA}$) [21]. Structural properties in equilibrium state viz. energy versus volume histograms, lattice parameters (a_0 , b_0 , c_0), bulk modulus (B_0) and its first order pressure derivative (B'_0) are calculated by fitting the total energy according to the Birch-Murnaghan's equation of state [16, 17] given by:

$$E_{total} = E_0(V) + \frac{B_0 V_0}{B'_0 (B'_0 - 1)} \left[B_0 \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B'_0} - 1 \right] \quad (12)$$

where, $E_0(V)$ and V_0 are the energy and volume at equilibrium. B_0 and B'_0 are the equilibrium bulk modulus and its first order pressure derivative.

The calculated lattice parameters (a_0 , b_0 , c_0), bulk modulus (B_0) and its first order pressure derivative (B'_0) are shown in Table 1, which show good agreement with available experimental values [18]. The energy versus volume curves for CeZn₂ has been shown in Fig. 1 which shows that the equilibrium energy (E_0) is minimum at volume $V_0 = 845.9967 \text{ eV}$ on which CeZn₂ is found to be stable in orthorhombic phase.

Table 1. Lattice parameters, a_0 , b_0 and c_0 ($\text{\AA}$), Bulk modulus, B_0 (GPa), Pressure derivative of bulk modulus, B'_0 (GPa) in equilibrium condition (at 0K) for CeZn₂ using GGA.

Compounds	a_0	b_0	c_0	B_0	B'_0
(Calculated)	4.629	7.539	7.494	64.53	4.55
Expt. [18]	4.635	7.540	7.501	---	---

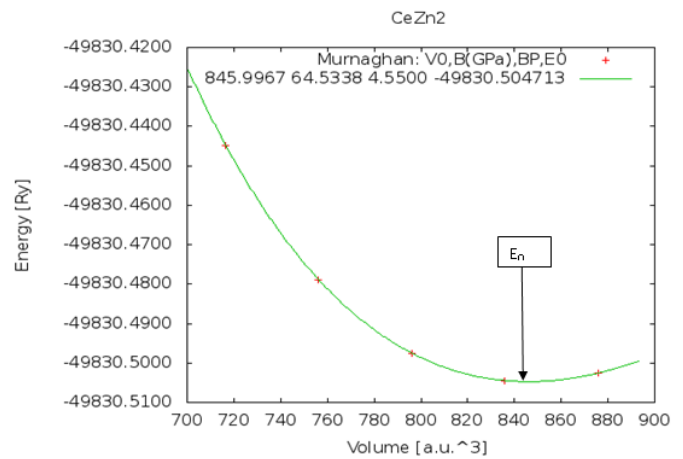


Figure 1. Variation of total energy with volume for CeZn₂ with GGA approximation.

3.2 Electronic properties

To investigate the bonding properties of CeZn₂, 3-D distribution of total valance charge density has been shown in Fig. 2. From figure it is clear that charge density distribution is spherically symmetric centered on Ce and Zn atoms, indicating ionic character. The d orbitals of Zn make up the most of this charge distribution due to high charge density around Zn. The calculated band structures for CeZn₂ along high symmetry directions in the Brillouin zone have been shown in Fig. 3. It can be seen from this figure that valence and conduction bands overlap significantly near the Fermi level (i.e. there is no band gap at the Fermi level), indicating metallic character of CeZn₂.

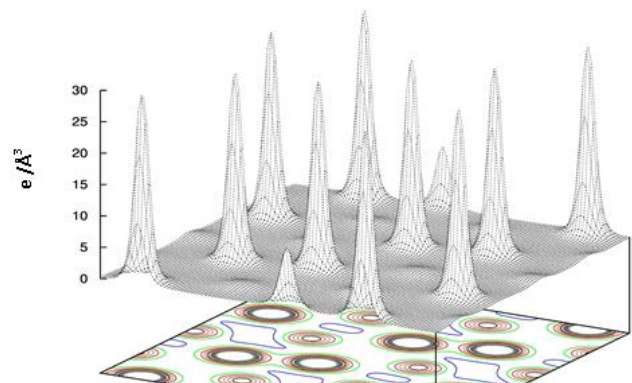


Figure 2. 3D-total valance charge density distribution for CeZn₂ with (100) plane.

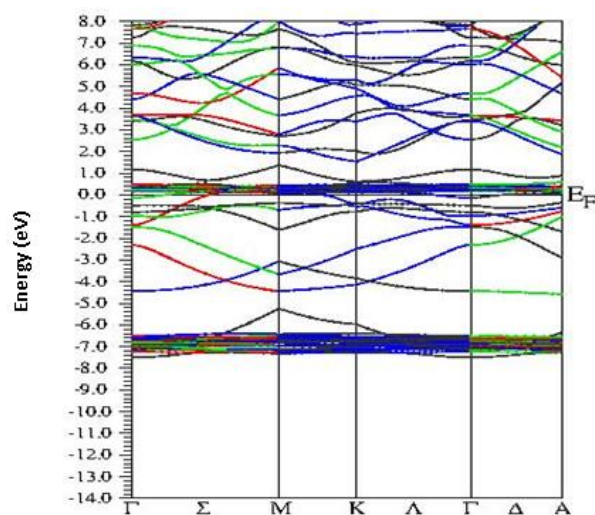


Figure 3. Electron dispersion curves along high symmetry directions in the Brillouin zone for CeZn_2

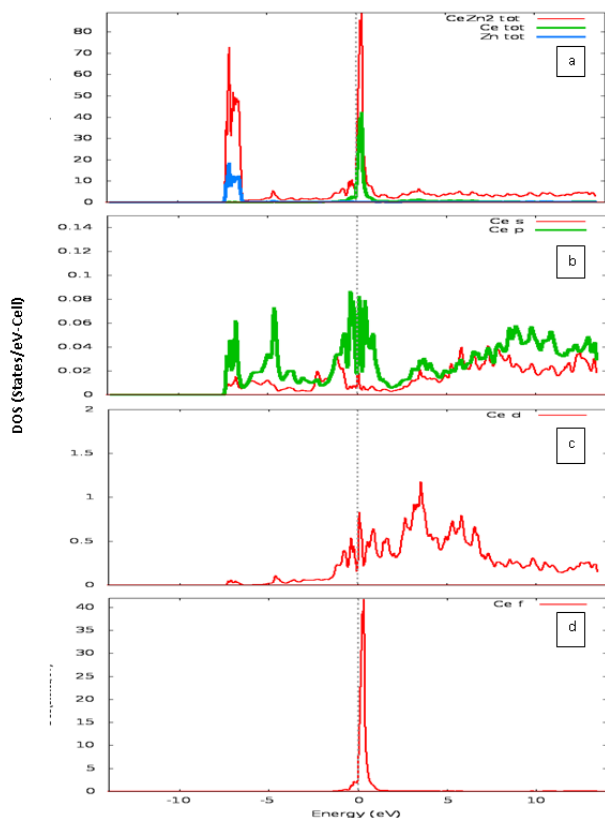


Figure 4. Calculated Total density of states for (a) CeZn_2 , Ce and Zn_2 and partial density of states for (b) Ce- "s", "p" (c) Ce-"d" (d) Ce-"f" orbital.

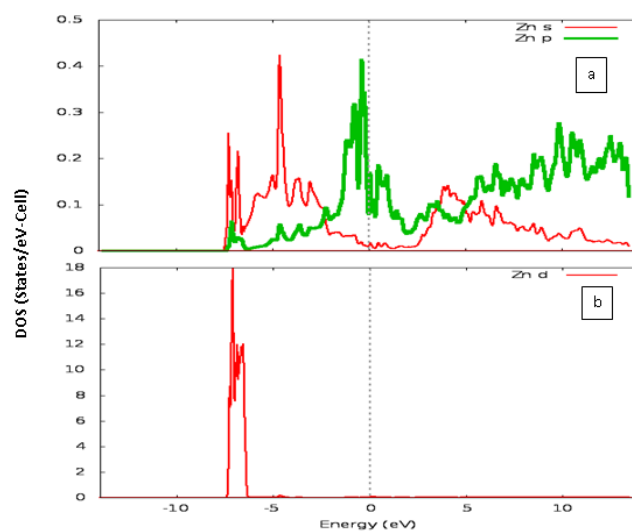


Figure 5. Calculated partial density of states for (a) Zn- "s", "p" (b) Zn-"d" orbital.

The total and partial density of states plots for CeZn_2 , Ce and Zn have been shown in Figures 4 (a) – 4 (d) and 5 (a, b). Figure 4 (a) displays the total density of states for CeZn_2 , Ce and Zn. Figs. 4 (b) – 4 (d) depict the partial density of states for s, p, d and f states of Ce, while Fig. 5 (a, b) shows the partial density of states s, p, d states for Zn. It is clear from Fig. 4(a) that most of the DOS lie in the energy range approximately between -7.5 eV to 0.0 eV. Strong hybridization is found to be existed between Ce-s and Ce-p states between -7.5 eV to Fermi level. From Fig. 4(d), it is clear that most of Ce-f states are found to be empty at around 0.5 eV above the Fermi level for conduction. A strong hybridization is also found between Zn-s and Zn-d states at around -7.5 eV in which Zn-d orbitals electrons are dominant (see Figure 5 (a) and 5 (b)).

IV. CONCLUSION

Full potential linearize potential augmented plane wave method using generalized gradient approximation (GGA). Calculated structural parameters are in consistent with available experimental data. Total valance charge density distribution histograms indicate the ionic character of CeZn_2 which is consequence of metallic character. Density of states plots show that "d" orbital electrons of Zn have dominant character below the Fermi level whereas Ce-f states are empty near the Fermi level for the conduction.

V. REFERENCES

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