



# First principles study of structural, electronic and elastic properties of lutetium mono-pnictides

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## ARTICLE INFO

### Article history:

Received 19 July 2010

Received in revised form 3 September 2010

Accepted 16 September 2010

Available online 13 October 2010

### Keywords:

Phase transition

Density functional theory

Band structure

Bulk moduli

Mono-pnictides

Lattice constant

## ABSTRACT

The structural, electronic, elastic and thermal properties of two lutetium mono-pnictides (LuAs and LuSb) have been studied using the density functional theory within the generalized gradient approximation. The calculations indicate that there is a structural phase transition from their ambient NaCl – ( $B_1$ ) to CsCl – ( $B_2$ ) structure at 56.7 and 25.2 GPa along with the volume collapse percentage of 3% and 5%, respectively. Structural parameters like lattice constant ( $a_0$ ), bulk modulus ( $B$ ) and pressure derivative of the bulk modulus ( $B'$ ) are presented. The calculated band structures indicate that  $B_1$  and  $B_2$  phase of these compounds are metallic. We have calculated the second order elastic constants for these compounds. We also compare the ground state ( $a_0$  and  $B$ ) and high pressure phase transition ( $P_t$ ) properties for three members of lanthanide series.

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## 1. Introduction

There is a growing interest in the study of electronic properties of rare earth (RE) pnictides; which is due to the variety of their magnetic and electrical properties despite their common rock salt structure [1]. These compound exhibit some unusual features in the electronics and magnetic properties and can be correlated with the existence of partially filled  $f$  electron shells of the lanthanide ions which are delocalized [2] and interact strongly with the lattice. Such behavior has been interpreted in terms of promotion of  $4f$  electron of rare earth ion to the  $5d$  conduction band and the mixing of  $f$  states with the  $p$  states of the neighboring ion. The majority of these compounds undergo the first order structural phase transition from the NaCl – ( $B_1$ ) type to CsCl – ( $B_2$ ) type structure at high pressure. So far as the structural properties are concerned, several pnictides of lanthanide group have been investigated by using high-pressure X-ray diffraction technique [3–6]. Besides the experimental studies, theoretical calculations based on density functional theory have been used to reproduce satisfactorily the experimental data and to obtain interesting properties in the case in which experimental measurements are yet to be done. Among these quantities, elastic constants represent a good test for estimating the quality of a theoretical approach [7,8].

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The electronic structures of lighter RE mono-pnictides have been investigated theoretically [9,10] in great details. Lanthanum, being the first member of the lanthanide series, a large number of theoretical as well as experimental studies is reported on lanthanum compounds [11,12]. Amongst the RE mono-pnictides, Gd mono-pnictides ( $GdX$ ,  $X = N, P, As, Sb, Bi$ ) are the simplest series because Gd is located in the centre of the series of the rare earth metal in the periodic table and has a half filled  $4f$  electron configuration. They are known to exhibit unusual electric [13] and magnetic [14,15] phenomena. The electronic properties of Gd mono-pnictides have been reported within the local spin density approximation (LSDA) [1,16].

The systematic theoretical study of high pressure phase transition and elastic properties of lutetium monochalcogenides ( $LuY$ ;  $Y = S, Se$  and  $Te$ ) were performed by Seddik et al. [17] by using first principles density functional theory. However, in the case of Lu-pnictides no theoretical work exists on the structural phase transformation except the experimental one reported by Shirotani et al. [4] who have used the X-ray diffraction technique to explore the high pressure properties [4,18]. Moreover, theoretical or experimental data on the electronic and thermal properties are not available for these compounds. However, the structural and elastic properties of LuSb have been predicted by us [29] by using two body interionic potential model. It is therefore, a timely effort to perform theoretical calculations and observe the effect of  $f$  electron on the calculated results with the other lanthanide compounds. Lu

being the last member of the lanthanide series with completely filled 4f shell, it is important to study the pressure behavior, electronic and elastic properties of these compounds.

In the present work, we report the high pressure behavior, electronic and elastic properties of two lutetium compounds, namely, LuAs and LuSb which crystallize in NaCl structure, by using density functional theory. The rest of the paper is organized as follows: In Section 2, we briefly describe the computational techniques used in this study. The most relevant results obtained for the structural, electronic and elastic properties of LuAs and LuSb are presented and discussed in Section 3. Finally in Section 4, we summarize the main conclusion of our work.

## 2. Computational details

The calculations were performed in the frame work of density functional theory. We have employed the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2 k code [7]. The exchange and correlation effects were treated using the generalized gradient approximation (GGA) in the scheme of Perdew et al. [19]. In order to achieve energy eigen values convergence, the wave function in the interstitial region were expanded in plane waves with a cut off  $K_{MAX} = 8.5/R_{MT}$ , where  $R_{MT}$  denotes the smallest atomic sphere radius and  $K_{MAX}$  gives the

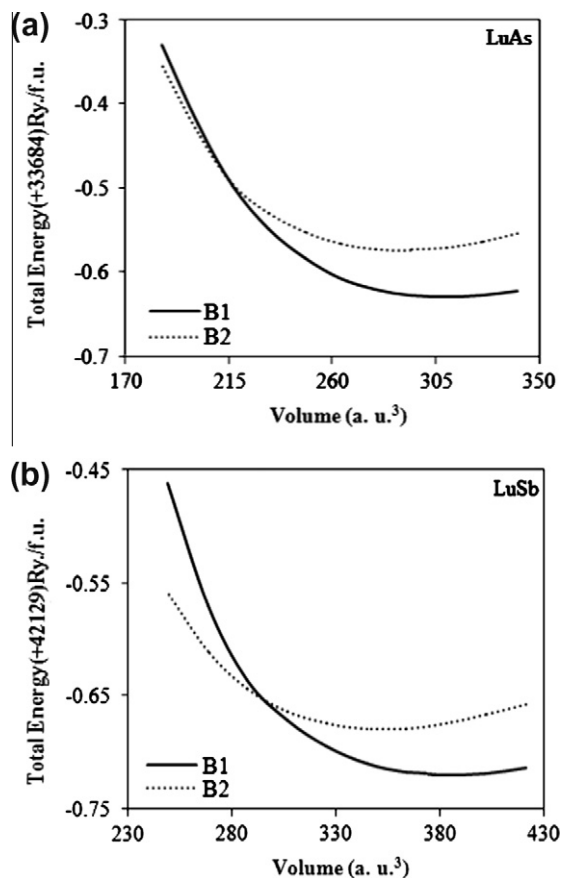


Fig. 1. (a and b) Total energy as a function of volume for (a) LuAs and (b) LuSb.

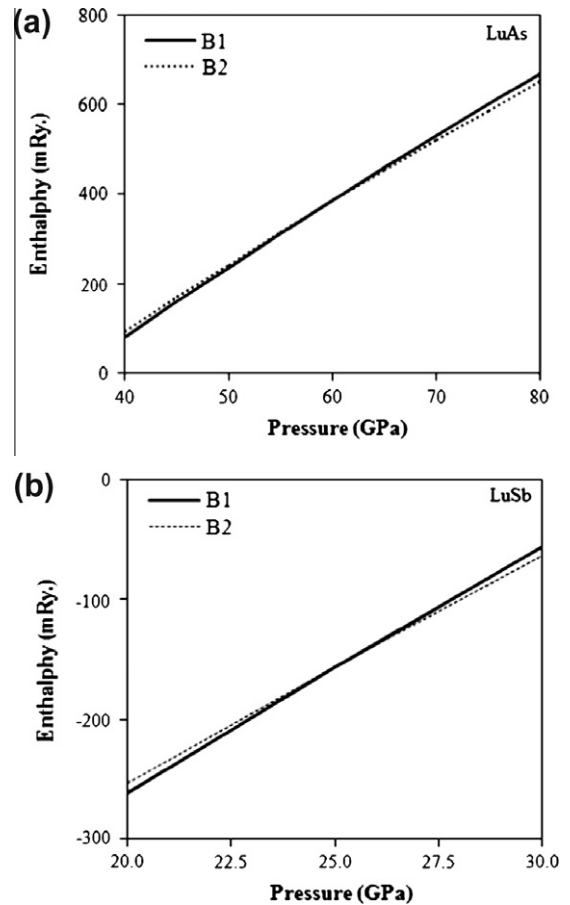


Fig. 2. (a and b) Variation of enthalpy as a function of pressure for (a) LuAs and (b) LuSb.

Table 1

Calculated lattice constant  $a_0$ , bulk modulus  $B$ , pressure derivative of the bulk modulus  $B'$ , density of states  $N(E_F)$ , phase transition pressure  $P_t$  and volume collapse% of LuAs and LuSb.

Solids	Structure	Work	$a_0$ (Å)	$B$ (GPa)	$B'$	$N(E_F)$ (State/eV)	$P_t$ (GPa)	Volume collapse (%)
LuAs	B <sub>1</sub>	Present	5.681	82.40	3.97	0.1801	56.7	3%
		Experimental	5.680 <sup>a</sup>	85 ± 3 <sup>a</sup>	5.9 ± 0.2 <sup>a</sup>	–	>57 <sup>a</sup>	–
		Other theory	–	–	–	–	–	–
	B <sub>2</sub>	Present	3.501	85.30	4.07	–	–	–
LuSb	B <sub>1</sub>	Present	6.113	58.04	3.75	0.2477	25.2	5%
		Experimental	6.040 <sup>d</sup>	53 ± 4 <sup>a</sup>	6 ± 0.8 <sup>a</sup>	–	>24 <sup>c</sup>	1% <sup>c</sup>
		Other theory	–	56.35 <sup>b</sup>	–	–	25.4 <sup>b</sup>	–
	B <sub>2</sub>	Present	3.719	66.40	4.11	–	–	–

<sup>a</sup> Ref. [4].

<sup>b</sup> Ref. [29].

<sup>c</sup> Ref. [18].

<sup>d</sup> Ref. [31].

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