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Research Article

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Structural parameters of LaS

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ABSTRACT

In this work, the structural properties of LaS are investigated using linear combination of atomic orbital method within density useful theory as inbuilt in CRYSTAL code. The exchange and correlation theme of Becke and PBE is employed. The structural properties are studied in terms of lattice constant, bulk modulus and its pressure derivative. All the results obtained were found to be in good agreement with the previous results.

Keywords: PBE, LCAO, BECKE, inter metallic compound, *ab-intio*

INTRODUCTION

Binary inter metallic compounds (LaX, X = S, Se or Te) show fascinating physical and structural properties. These properties are due to the interaction between the conduction electrons and the 4f electrons. Most of the compounds shows the structural phase transformation from B1 (NaCl) to B2 (CsCl) structures at high pressure. At, normal pressure the structure of these compounds is NaCl. In addition to this, these compounds show the phenomena of superconductivity also. Therefore an attempt has been made to investigate the structural parameters of LaS.

Theoretical details

In the present work, an attempt is made to investigate the structural properties of LaS using density functional theory as inbuilt in CRYSTAL [1] code. The local functions of La and Se were constructed by taking the help from Gaussian basis set [2]. For constructing Hamiltonian the exchange and correlation function of Becke and PBE were used respectively. This method is best suitable for binary compounds [3-5].

RESULTS AND DISCUSSION

LCAO method have been used to calculate the total energies for structures of LaSe on a volume set. Variations in the net energy relative to the volume for both compounds in the two phases are specified in the Figures 1 and 2. The points showing the calculated energy and the continuous lines show the fitted curves according to the equation Brich Murnaghan equation of sate. The calculated structural parameters of LaSe in B1 and B2 phases are listed in Table 1. It is evident from the figures that the B1 phase is energetically favorable phase for both compounds because its energy is lower than than B2 phase.

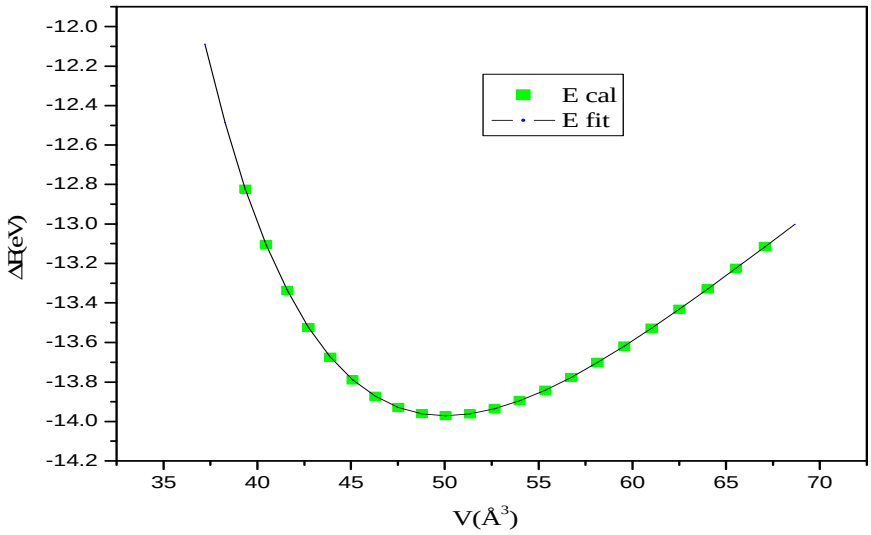

Figure 1. E vs V for LaS of B1

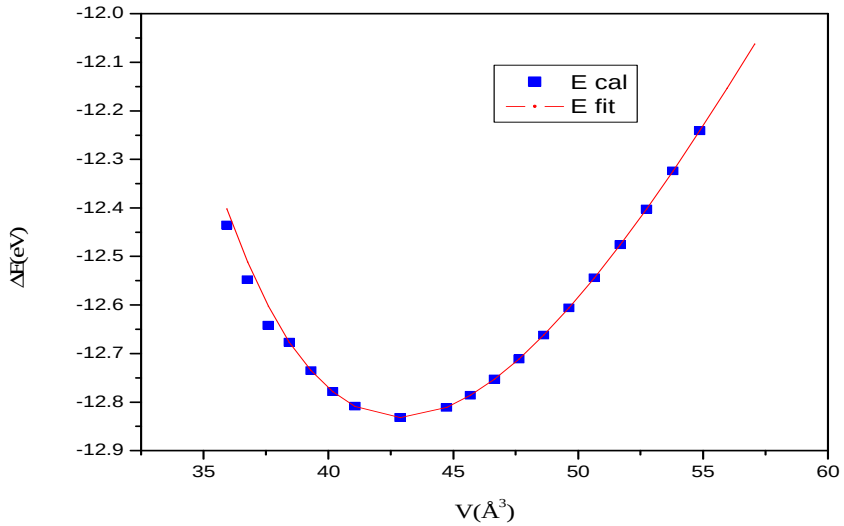

Figure 2. E vs V for LaS B2

Table 1. Calculated and experimental lattice parameter (a), bulk modulus (B0) and its pressure derivatives (B0') for LaS

		Present	Experimental	Other Calculations
LaS				
B1	**a (Å)**	5.85	5.85[5]	5.86 [6] , 5.73[7], 5.85[8]
	B_0 (GPa)	93	89 [5]	107[7], 86[9],87.8[5]
	B_o'	5.89	6.5[5]	-
B2	**a (Å)**	3.5	-	3.30[7]
	B_0 (GPa)	88.56	-	228[7]
	B_o'	4.5	-	-

CONCLUSION

In summary, the first-principles calculations have been done using the LCAO method in combination with GGA to study the structural properties of the LaS
The main conclusions are:
(i) The total energy calculations show that the stable phase is B1.
(ii) B2 phase is more compressible than B1

The results obtained are in good agreement with the previous investigations.

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