Phase transition in LaS

N. Munjal[1*], K. Kaur[1], and G. Sharma[2]
[1]Department of Physical Science, Lovely Professional University, Punjab, India
[2]Department of Pure and Applied Physics, University of Kota, Kota
***Corresponding author: E-Mail: neha.18869@lpu.co.in**

ABSTRACT

In this work, the phase transition in LaS is 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 results obtained are in good agreement with the previous investigations

KEY WORDS: PBE, LCAO, BECKE, inter metallic compound, LaS.

1. INTRODUCTION

Metals are from one of the technologically important class of materials due to their ductility and high electrical and thermal conductivities. The investigations of the properties of the rare-earth mono chalcogenides have been a challenge for the researchers as it is very difficult for the researchers to fabricate them into the single phase. But the advancement of first principles calculations have open the path for the researchers. Therefore, in this research work an attempt has been made to compute the phase transition in the binary inter metallic compound LaS.

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

Results and discussion: The Gibbs free energy (G = U + PV-TS) is used for calculation of the transition pressure. Since all our density functional calculations are performed at T = 0 K, Gibbs free energy reduces the enthalpy H = E_o + P V. A particular pressure, the thermodynamically stable phase is the one that has the enthalpy smaller. The transition from one phase to the high-pressure phase occurs when the enthalpy curves coincide. In LaS, B1-B2 transition occurs to 24.34 GPa. The comparison of the result with previous calculations is shown in Table 1.

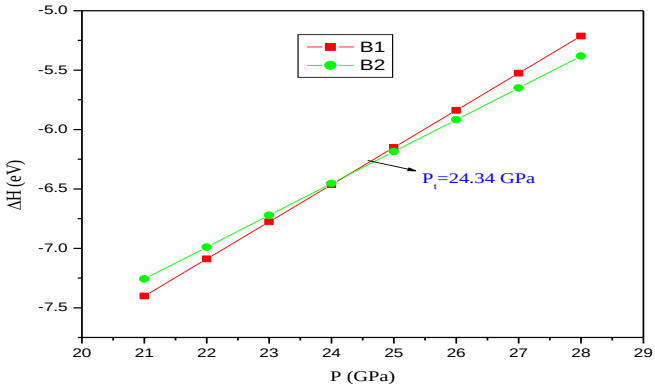

Figure.1. Enthalpy vs pressure

Table.1. Calculated and experimental Phase Transition for LaS

Present	Experimental	Other Calculations
24.34	-	29.3 (Vaitheeswaran G, 2002), 25.5 (Varshney D, 2004), 24.9 (Vaitheeswaran, 2007)

2. CONCLUSION

The LCAO method have been employed for determining the phase transition in LaS. It is found that phase transition occurs from B1 to B2 at 24.34 GPa. The obtained result is close agreement with previous calculations.

REFERENCES

Dovesi R, Saunders VR, Roetti C, Orlando R, Zicovich-Wilson CM, Pascale F, Civalleri B, Doll K, Harrison NM, Bush IJ, Arco D, Llunell M, CRYSTAL06 User's manual, University of Torino, Torino, 2006

Munjal N, Bhakri K, and Sharma G, First principle study of phase transition in CaO, JOCPR, 7 (7), 2015, 289-291

Munjal N, Sharma G, Vyas V, Joshi KB, Sharma BK , Ab-initio study of structural and electronic properties of AlAs, Phil. Mag., 92 (24), 2012, 3101.

Vaitheeswaran G, Kanchana V, and Rajagopalan M, Theoretical studies on the high pressure phases of Lanthanum monochalcogenides, J. Phys. Chem. Solids, 64, 2003, 15.

Vaitheeswaran G, Kanchana V, Heathman S, Idiri M, Le Bihan T, Svane A, Delin A, and Johansson B, Elastic constants and high-pressure structural transitions in lanthanum monochalcogenides from experiment and theory, Phys. Rev., 75, 2007, 184108

Varshney D, Kaurav N, Sharma P, Shah S, and Singh R.K, Structural phase transition of Lanthanum monochalcogenides induced by hydrostatic pressure, Phys. Status Solidi B, 241, 2004, 3179.

www.tcm.phy.cam.ac.uk.