

**STUDY OF STRUCTURAL PHASE TRANSFORMATION IN LaSe****Munjal N**

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ARTICLE INFO**Article History:**Received 22nd May, 2016Received in revised form 28^h June, 2016Accepted 15th July, 2016Published online 28th August, 2016**ABSTRACT**

In this work, the density functional theory as inbuilt in CRYSTAL code is used to study the phase transition in LaSe. The Becke and PBE schemes are used for exchange and correlation. The obtained results are in close proximity with the previous studies.

Key words:

PBE, LCAO, BECKE, inter metallic compound, LaSe.

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INTRODUCTION

Rare earth compounds have received the great attention because of their interesting properties in the field of non linear optics, glass making, lasers etc. Now a days, the applications in spintronics is also coming into existence. Therefore, here an attempt has been made to evaluate the transition of structure from B1 to B2 for the LaSe compound.

Theoretical details

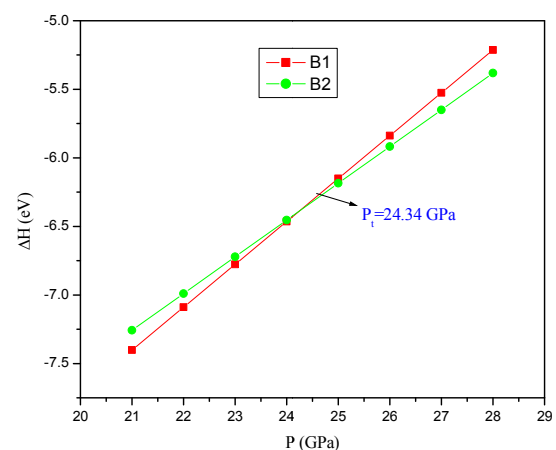
The work focuses on the phase transition in LaSe from NaCl structure to CsCl structure using linear combination of atomic orbital method [1]. The Gaussian basis set are used for contracting the local functions of La and Se [2]. For building Hamiltonian the exchange and correlation function of Becke and PBE were used respectively. The method is appropriate for binary compounds.

RESULTS AND DISCUSSION

The enthalpy is used for $H = E_0 + P V$ is used for calculating the pressure at which the transition takes place from one structure to the other. The transition from one structure to the high-pressure structure occurs when the curves of enthalpy coincides. In LaSe, the transition occurs at 13.05 GPa. The results are compared in Table 1.

Table 1 Calculated and experimental Phase Transition for LaSe in GPa

Present	Experimental	Other Calculations
13.05	-	12.4[7], 12.7[8], 12[9], 21[10]

**Figure 1** Enthalpy vs pressure**CONCLUSION**

The phase transition in LaSe occurs from B1 to B2 at 13.05 GPa. The obtained result is in close agreement with previous calculations.

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