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Ab-initio Study of Phase Transition in LaSe

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ABSTRACT

In this work, the density functional theory as inbuilt in CRYSTAL code is use to study the phase transition in LaSe The exchange scheme of Becke and correlation theme of PBE is employed. The results obtained are in good agreement with the previous investigations

Keywords: PBE; LCAO; BECKE; Inter metallic compound; LaSe

INTRODUCTION

Rare earth compounds have received the great attention because of their interesting properties in the field of nonlinear optics, glass making, lasers etc. Now a days, the applications in spintronics is also coming into existence. Therefore, in this research work an attempt has been made to compute the phase transition in the binary inter metallic compound LaSe.

THEORETICAL DETAILS

In the present work, an attempt has been made to investigate the phase transition in LaSe from NaCl structure to CsCl structure using linear combination of atomic orbital method [1]. 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 [3-6].

RESULTS AND DISCUSSION

The enthalpy is used for $H = E_o + P V$ is used for calculating the pressure at which the transition takes place from one structure to the other. The transition from one phase to the high-pressure phase occurs when the enthalpy curves coincide. In LaSe, B1-B2 transition occurs to 24.34 GPa. The comparison of the result with previous calculations is shown in Table 1 and Figure 1**.**

Table 1: Calculated and experimental Phase Transition for LaSe in GPa

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]

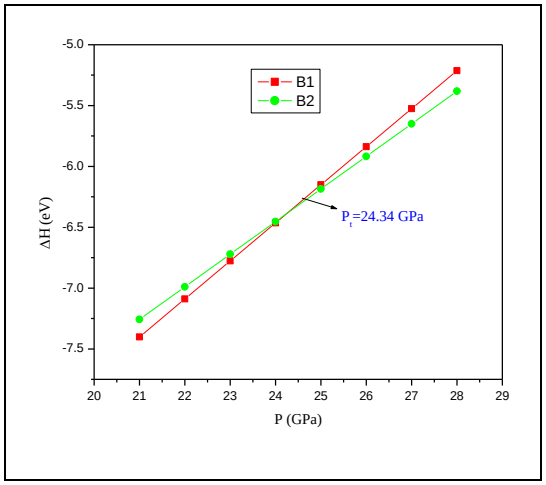

Figure 1: Enthalpy vs pressure

CONCLUSIONS

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

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