



# STRUCTURAL AND VIBRATIONAL PROPERTIES OF LEAD-LITHIUM ALLOYS: A FIRST PRINCIPLES STUDY

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## Prologue

Lead-Lithium (Pb-Li) alloy in its eutectic composition is one of the promising candidates to be used as liquid blanket in fusion reactor. Helium cooled Lead Lithium (EU-HCLL), Dual cooled Lead Lithium (US-HCLL), Indian LLCB are some of the concepts being explored worldwide for future fusion reactor [1]. In this scenario, the characterization of Pb-Li alloy becomes important to gainfully understand its underlying physical/structural behavior. In literature, it is found that, lot of works have been devoted to calculate the phase diagram of Pb-Li alloy at various compositions. Contrarily, the prerequisite for the Pb-Li alloy characterization such as its ground state property is widely missing in literature. Hence, present work is an attempt to fill the gap by calculating the structural and vibrational properties of Pb-Li alloy.

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## Progress made so far by the community

The work on Lead-Lithium system is mostly devoted to study of properties in liquid phase and study of phase diagram.

Study is also performed for properties related to eutectic composition.

However, the study of properties in solid phase is still less and we believe that for the complete theoretical characterization, study of properties in solid phase is also required.

Thus, in the present work, we report the results of our theoretical study of various structural and vibrational properties of Pb-Li.

## Next steps/ Critical Issues

We are working on various physical properties of Lead-Lithium.

Our aim is to develop a cross potential for Pb-Li as no such potential is available in literature.

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