

# Structural and Vibrational Properties of Lead-Lithium Alloys: A First Principles Study

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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 the present paper, we report the results of our computer experiments on structural and vibrational properties of Pb-Li. Present work is performed using plane wave pseudopotential density functional theory within generalized gradient approximation (GGA). Calculations of various structural properties at ambient condition ( $T, P = 0$ ) are performed using Quantum ESPRESSO package. Further, phonon frequencies along major symmetry directions are also calculated using density functional perturbation theory. Three independent elastic constants are also calculated for both the compensating structures namely Rhombohedral and CsCl type. Calculations of equation of state at elevated temperatures suggest that Pb-Li is a soft material undergoing large volume change with pressure. Further, some thermodynamic properties at elevated temperatures are also reported.

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