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Determination of mechanical, structural and thermodynamic properties of half-heusler compound (ZRPDPB) in solid state physics

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In this work, the structural, mechanical and thermodynamic properties of Zirconium Lead Palladium ate (ZrPdPb) were investigated by the first-principle calculations using Quantum Espresso that implements Density Functional Theory. The results indicate that all Half-Heusler compounds are narrow-gap semi-conductors. The results of Young's modulus, elastic constants C_{11}, C_{12} and C_{44}, Shear modulus, and Lattice constants, Bulk modulus and pressure derivative which constitute the mechanical and structural properties respectively of ZrPdPb are in good agreement with the results in literature. The thermodynamic properties of ZrPdPb such as Heat capacity, internal energy, entropy, free energy, Debye temperature etc. were calculated using Quantum Epsresso.It is seen that at room temperature i.e. 300k, the internal energy is 23.15kJ/(mol/K), and the heat capacity is 72.27kJ/(mol/K) .The Debye temperature is found to be 365.3K . From 500k and above, the heat capacity approaches an asymptotic value of 37J/mol/K, and obeys Dulong-Petit law which states that at high temperature Specific heat capacity of a substance remains constant. Also, at sufficiently low temperature, the specific heat capacity is proportional to T_3. The mechanical properties ZrPdPb show that the material is not stable under heavy vibration. Suggestions were made to improve the mechanical and thermodynamic properties. Other properties like the magnetic and optical properties of ZrPdPb should be studied.

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