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FIRST PRINCIPLES STYDY OF STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF TERNARY HYDRIDE SrPdH3

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Abstract

We have applied the full-potential linearized augmented plane wave (FP-LAPW) method to study the structural, elastic and electronic properties of the ternary hydride SrPdH3. We have employed the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange and correlation potential.

The equilibrium lattice constants and the bulk modulus and its pressure derivative are calculated and compared with available experiment and theoretical results.

we have also predicted the elastic constants, Anisotropy factor (A), Young's modulus (E), Poisson ratio (υ), shear modulus (G), sound velocities (v_l, v_t, v_m) and Debye temperature (θ_D).

The contribution of the different bands was analysed from total and partial density of states curves. Our calculation of band structure shows an indirect band gap.

Key words: *DFT, FP-LAPW, Dos, perovskite, hydride*

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