

Density functional (DFT), Study of the Structural and Phase Transition of ThC and ThN: LDA vs GGA Computational

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Abstract : The present paper deals with the computational of structural and electronic properties of ThC and ThN compounds using density functional theory within generalized-gradient (GGA) approximation and local density approximation (LDA). We employ the full potential linear muffin-tin orbitals (FP-LMTO) as implemented in the Lmrt code. We have used to examine structure parameter in eight different structures such as in NaCl (B1), CsCl (B2), ZB (B3), NiAs (B8), PbO (B10), Wurtzite (B4), HCP (A3) β Sn (A5) structures. The equilibrium lattice parameter, bulk modulus, and its pressure derivative were presented for all calculated phases. The calculated ground state properties are in good agreement with available experimental and theoretical results.

Keywords : DFT, GGA, LDA, properties structurales, ThC, ThN

Conference Title : ICCP 2022 : International Conference on Computational Physics

Conference Location : Paris, France

Conference Dates : December 29-30, 2022