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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) apraximation and local density approximation (LDA). We employ the full potential linear muffin-tin orbitals (FP-LMTO) as implemented in the Lmtart 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) βSn (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
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