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Atomistic Study of Structural and Phases Transition of TmAs Semiconductor, Using the FPLMTO Method

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Abstract : We report first-principles calculations of structural and magnetic properties of TmAs compound in zinc blende(B3) and CsCl(B2), structures employing the density functional theory (DFT) within the local density approximation (LDA). We use the full potential linear muffin-tin orbitals (FP-LMTO) as implemented in the LMTART-MINDLAB code (Calculation). Results are given for lattice parameters (a), bulk modulus (B), and its first derivatives(B') in the different structures NaCl (B1) and CsCl (B2). The most important result in this work is the prediction of the possibility of transition; from cubic rocksalt (NaCl)→ CsCl (B2) (32.96GPa) for TmAs. These results use the LDA approximation.

Keywords : LDA, phase transition, properties, DFT
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