Pressure induced structural phase transition and lattice dynamics in thallium-V compounds

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Abstract: Most of the III–V type semiconductor materials have been subjected to intensive theoretical and experimental studies for many years. This is mainly due to their interesting electronic properties, their use in semiconductor devices and the relative ease with which such compounds can be synthesized. In the present study, an effective interionic interaction potential (EIOP) is developed to investigate the pressure induced phase transitions and lattice dynamics of the Zincblende thallium-V compounds: TlAs, TlP and TlN. The long range Coulomb, van der Waals (vdW) interaction and the short-range repulsive interaction up to second-neighbor ions within the Hafemeister and Flygare approach with modified ionic charge are properly incorporated in the EIOP. The vdW coefficients are computed following the Slater-Kirkwood variational method, as both the ions are polarizable. The estimated value of the phase transition pressure (Pt) and the magnitude of the discontinuity in volume at the transition pressure are consistent as compared to the reported data. The vast volume discontinuity in pressure volume phase diagram identifies the structural phase transition from Zincblende (B3) to NaCl (B1) structure. Phonon dispersion spectra are derived using EIOP and compare with the previous report.

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