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# New High-Pressure Phase and Properties of Thallium under High Pressure: An ab initio investigation

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In the recent work, we have demonstrated the high-pressure phase transitions of a heavy element thallium (Tl). The known first phase transition from h.c.p. to f.c.c. is initially investigated by various relativistic levels and exchange-correlation functionals as implemented in FPLO method, as well as scalar relativistic scheme within PAW formalism. The electronic structure calculations are interpreted from the perspective of energetic stability and electronic density of states. The full relativistic scheme (FR) within L(S)DA performs to be the scheme that resembles mostly with experimental results with a transition pressure of 3 GPa. The s-p hybridization and the valence-core overlapping of 6s and 5d states are the primary reasons behind the f.c.c. phase occurrence. The electron-phonon coupling and the superconducting critical temperature (Tc) as a function of pressure are evaluated. The findings show that both Tc's of h.c.p. and f.c.c. phases decrease with increasing pressure and the Tc of f.c.c. phase approaches zero at 30 GPa. We have also uncovered the unusual distortion in face-centered cubic (f.c.c.) phase, namely the body-centered tetragonal (b.c.t) phase, of Tl which is induced by the high pressure at approximately 83 GPa. This prediction has been confirmed by experimental results of using an angle dispersive X-ray diffraction technique. The reversible b.c.t. ⟶ f.c.c. phase transition of Tl is predicted around 800 GPa. Our finding provides the extension of the phase diagram of Tl under high pressure as h.c.p⟶f.c.c.⟶b.c.t⟶ f.c.c.

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