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Structural phase transition of binary compounds of TlX (X = N, P, As) under high pressure : An *ab initio* Study

Thursday, May 21, 2015 8:00 AM (3 hours)

In this work, density functional theory (DFT) has been performed to investigate high-pressure phase transitions of TlX (X = N, P, As). Both standard GGA and LDA functionals with norm-conserving pseudopotential are used to compare each other in recent work which the calculation results are reported in form GGA (LDA). Based on the previous theoretical predictions, B3-to-B1 (B4-to-B1 for TlN) are reinvestigated initially, as well as the other candidates with crystal structure of *Cmcm*, *P4/mmm*, *Cmmm*, and B2-type structure are undertaken for comparing energetically to predict the high-pressure phases in these compounds. It reveals that TlN and TlP transform to B1 at 19 (16) and 28 (10) GPa, by compressing B4 and B3, respectively. The reduction volumes are approximately 14.8 (15.2) % and 14.7 (16.4) % for TlN and TlP, respectively. Moreover, B2-type is predicted at 340 (395) GPa for TlN, and at 97.5 (81) GPa for TlP with passing through *P4/mmm*. In TlAs, B3-type structure does not undergoes to B1-type. But it could possibly transform to *Cmcm* and *Cmmm* structure at which is different with previous predictions.

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