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# Effect of 6.25 at.% Ta on TiPtCo Shape Memory Alloy

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In this study, the phase stability of B2 and B19 Ti50Pt43.75-xCoxTa6.25 structures using ab initio density functional theory approach was investigated. Their structural, vibrational and mechanical properties were determined to show their stability. The supercell approach was employed to substitute Pt with Ta on the TiPtCo and evaluate the stability of the structures. The calculated heats of formation predicted Ti50Pt37.50Co6.25Ta6.25 to be the most stable structures as compared to other concentrations for both B2 and B19 systems. The calculated elastic properties show that TiPtCoTa is mechanically stable at different concentrations of Co. Moreover, the temperature dependence was also calculated to predict the possible transformation.

## Apply to be considered for a student ; award (Yes / No)?

Yes

## Level for award;(Hons, MSc, PhD, N/A)?

PhD

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