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## The study of Zr and Nb alloyed on the beta-Ti for bio-medical applications: first principle approach.

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### Abstract:

Titanium alloys have been used in the bio-medical industry since the 1800s. They are incredibly important among bio-medical implants because of their high strength and resistance to fatigue deterioration. Recently, the development of non-toxic, more biocompatible and allergy-free components has been of outmost importance. The purpose of this study was to use first principle approach to investigate the effect of alloying Ti with Nb and Zr to improve the mechanical properties of Ti alloys for use in human implantations. This is attributed to the  $\beta$  phase stabilization ability and high bio compatibility of these transitional element. Increasing Zr and Nb concentrations on the Ti stabilized the alloy with a lower young's modulus compared to that of pure Ti.

Key words: Titanium alloys, Heats of formation, Lattice parameters, Density of states, Elastic properties.

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

Yes

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

Hons

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