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Investigation of beta Ti-Mo phase stability employing the first principle approach

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The improvement for load bearing dental and orthopedic implants of Titanium based alloys have become significant in the medical industry, due to the increase of knee and hip replacement amongst younger individuals and the deterioration of body parts by increasing human age. Hence the need for developing low modulus Ti-based alloys with biocompatible properties and low elastic modulus close to the bone. This study aims to investigate the stability of Ti-based alloys for biomedical applications using the first-principles approach. The stability of beta Ti100-xMox (x=0-10) alloys was investigated with respect to their equilibrium lattice parameters, elastic constants and the density of states. The study employed the density functional theory within the generalized gradient approximation. Addition of the alloying element was achieved employing the visual crystal approximation embedded in CASTEP. Interestingly, the Mo addition stabilizes the beta phase with an increasing C' moduli and the density of states suggest that the phase is being stabilized at a higher content of Mo (20 at.%).

Apply to be
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Yes

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

MSc

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