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First principle' study of the properties of the Titanium based alloys (Ti doped with Mo, Mg, Zr, Ta and Si) for biomedical applications

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Introduction-□–Ti alloys presented excellent human implantation properties from research over the past 7 decades.
Aim-The aim of the study is to investigate the three main selected properties of Ti-based alloys, which include the structural stability, mechanical and elastic properties doping with Mg, Mo, Zr, Ta and Si for biomedical applications using the First Principle' Approach.
Method-The investigation was performed with the use of a computer simulation software, CASTEP code which contains the virtual crystal approximation (VCA) that applies the ab-initio total energy calculations belonging to the density functional theory (DFT) via the route
of plane wave pseudopotential calculations for Kohn-Sham equations, with the help of Perdew-Burke-Ernzerhof (PBE) of the generalized gradient approximation (GGA).
Results-The fermi level of the PDOS of Ti-Si alloy is located slightly on the edge of the d-orbital. A pseudo gap appears near the fermi level in the PDOS graph of Ti-Mo alloy indicating a stabilized covalent bond. For the PDOS of Ti-Ta alloy, weaker bonds are shown which elaborates less stability. The fermi level is at the far edge of the d-orbital therefore showing weaker stability.
Conclusion-The results with the experimental values thus indicating that the investigation wasindeed successful.

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

yes

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

MSc

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