
Contribution ID: **304** Type: **Poster Presentation**

# The study of the properties of Titanium based alloys for biomedical applications using the First Principle' approach.

*Thursday, 6 July 2023 16:27 (1 minute)*

ABSTRACT
Titanium (Ti) and its alloys have been widely used as implant materials due to their outstanding mechanical characteristics and biocompatibility. Some of the applications includes orthopedic, and endoderm surgeries etc. However, there is a great concern regarding the difference in the implant material's Young's modulus and that of natural bone. With prolonged use, Ti alloys releases dangerous ions to the human body hence the need to improve the Young's moduli of these alloys. The aim of the study is to investigate the structural and mechanical stability of Ti-Mg-Si alloys using first principle approach. The elastic properties and the Density of States (DOS) of the alloys were determined by the first-principle calculations based on the Density Functional Theory (DFT) using Cambridge Serial Total Energy Package (CASTEP) and the results were compared with the available experimental results. Cubic Ti-Mg-Si tends show a rise in the density of states peak near the fermi line. In conclusion Mg contribution to the structure Ti-Mg-Si leads to a formation of a metallic bond and increased elasticity which confirms the mechanical and structural stability.

Key words: Properties of Titanium based alloys, Structural and Mechanical stability of Ti-Mg-Si alloys, DFT, First-Principle.

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

yes

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

MSc

**Primary author:** MABEBA, Kobe (Student)

**Co-authors:** Prof. SITHOLE, Enoch (Sefako Makgatho Health Sciences University); Dr MODBA, Rosinah (CSIR)

**Presenter:** MABEBA, Kobe (Student)

**Session Classification:** Poster Session 2

**Track Classification:** Track G - Theoretical and Computational Physics