Contribution ID: **355** Type: **Poster Presentation**

First-principles study of Hf- and Cu-doped Ti-Ni-Mo shape memory alloys: structural stability and mechanical properties for biomedical applications.

Titanium-based shape memory alloys (SMAs) are valuable for biomedical applications due to their mechanical stability and biocompatibility. However, their clinical performance is limited by ion release, stress shielding effects due to bone-implant stiffness mismatch, toxicity risks, and the need for optimized phase stability. This study aims to improve the Ti-Ni-Mo alloy's performance by investigating how replacing some Ni atoms with small amounts of Hf and Cu affects its properties. DFT first-principle calculations were performed to examine the impact of introducing Hf and Cu into Ti-Ni-Mo on its thermodynamic, mechanical, and electronic properties, aiming to optimize mechanical strength alongside biological compatibility for prolonged implant functionality. These properties include heats of formation, elastic constants via Born criteria, elastic moduli from the Voigt-Reuss-Hill method, and density of states (DOS) analysis. The density of states plots analysis indicated that Hf doping improves Ti-3d orbital hybridization improving phase stability. While Cu doping redistributes electron density around Ni atoms, enhancing ductility. These findings enable systematic development of Ti-based shape memory alloys, where controlled doping achieves the crucial objectives of thermodynamic, mechanical, electronic properties and biocompatibility for medical implants.

Apply for student award at which level:

PhD

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary author: Ms MNISI, Velile (Sefako Makgath health science university)

Co-authors: SITHOLE, Enoch; MODIBA, Rosinah

Presenter: Ms MNISI, Velile (Sefako Makgath health science university)

Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials