Contribution ID: **386** Type: **Poster Presentation**

Exploring Surface Stability in Titanium Nickel Using DFT

Titanium Nickel (TiNi) alloys are widely used in biomedical and aerospace applications due to their unique shape memory effect and superelastic properties. However, their susceptibility to corrosion in aggressive environments limits their long-term performance and reliability. Understanding the surface stability of TiNi is crucial for developing strategies to enhance corrosion resistance and optimise its functionality in various applications such as biomedical devices and robotics. This study employs density functional theory (DFT) calculations to investigate the surface stability of TiNi alloy, focusing on the (100), (110), and (111) surfaces. The calculations revealed that the (110) surface has the lowest energy illustrating stability. The PDOS results corroborate the enhanced stability of the (110) surface, showing a more favourable electronic configuration compared to the (100) and (111) surfaces. Additionally, we calculated the work function for each surface and it was observed that the (110) surface has higher work function than the (100) and (111) surfaces, suggesting that the (110) surface is less reactive and more stable. This data will provide insights into the stability, reactivity, and potential applications of TiNi in catalysis and electronic devices.

Apply for student award at which level:

MSc

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary author: CHAUKE, Vukosi (University of Limpopo)

Co-authors: CHAUKE, Hasani Richard (University of Limpopo); Dr TSHWANE, David (CSIR); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: CHAUKE, Vukosi (University of Limpopo)

Session Classification: Poster Session