Contribution ID: **101** Type: **Poster (sponsored)**

Computational modelling of TiPd-Ir high temperature shape memory alloys.

HPC content
Stability of the B2 TiPd-Ir high-temperature shape memory alloys calculations were achieved by utilizing various codes in the Medea environment at the CHPC.
The structural, thermodynamic, phonon dispersion curves and elastic properties were achieved by utilizing the VASP code, CASTEP code was utilized to study the density of states of the compound.
Application code: VASP, CASTEP
Problem size: 16 – 1024 atoms
Core count: 48
Computational challenges: no challenges so far.

Presenter Biography

Ms Ramogohlo Diale is a second year Masters student at University of Limpopo. She received her Hons in Physics (2017) from the University of Limpopo (UL) with the tittle: "computational modelling of Titanium Aluminium alloys and the effect of Iridium alloying". She is currently studying "computational modelling studies of martensitic transformation of TiPd shape memory alloys".

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