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# Computational modelling of temperature dependence of Ti<sub>50</sub>Pt<sub>50</sub> shape memory alloys

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## Abstract content <br>   (Max 300 words)<br><a href="http://events.saip.org.za/getFile.py/a target="_blank">Formatting &<br>Special chars</a>

Shape memory alloys (SMAs) have attracted considerable attention and interest in recent years in a broad range of commercial demands due to their unique and superior thermodynamic properties. Their shape memory effect and pseudoelasticity has drawn significant interest in commercial development. SMAs are a group of metallic alloys with unique characteristics, have the ability to return to their original form or shape or size when exposed to a memorisation process between martensite and austenite phase, which is temperature dependent. The first-principle density functional theory was employed to investigate the temperature effect of equiatomic B2, B19 and B19' TiPt SMAs. We observed a martensitic transformation when Ti 50 at.% Pt is exposed to extreme temperatures of up to 1573K. However, the temperature dependence of TiPt shows potential martensitic change for B19 and B19' as compared to B2 phase. Moreover, molecular dynamics studies of martensitic transformation temperature for titanium platinum alloys were carried out using CASTEP code. The NPT ensemble was used to determine the properties of these systems and we found good comparisons with recent experimental work.

## Apply to be<br> considered for a student <br>   award (Yes / No)?

yes

## Level for award<br> (Hons, MSc, <br>   PhD)?

MSc

## Main supervisor (name and email)<br>and his / her institution

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## Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

Yes

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