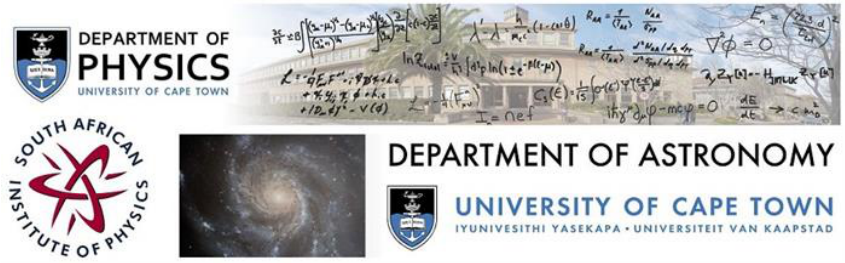

Contribution ID: **393** Type: **Poster Presentation**

Beneficial effects of Cobalt on ZrNb alloy using density functional theory and virtual crystal approximation.

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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Zirconium and its alloys are presently being developed as cladding materials due to their high temperature application and corrosion resistance. Density functional theory (DFT) and Virtual Crystal Approximation (VCA) were used to investigate the influence of Co addition on the thermodynamic, electronic and mechanical properties of ZrNb alloys. Where a lesser amount of atomic percent Co has shown to have a beneficial effect on the ZrNb alloy suitable for industrial applications. This was verified through the obtained results which are reporting on the equilibrium lattice parameters, heats of formation, elastic properties and the density of states. The investigated properties are evaluated to mimic the stability trend in the competing phases of Zr₉₇Nb_{3-x)}Co_x , Zr_{97.5}Nb_(2.5-x)Co_x , Zr_{98.1}Nb_(1.9-x)Co_x , Zr_{98.5}Nb_(1.5-x)Co_x , Zr_{98.8}Nb_(1.2-x)Co_x, and Zr₉₉Nb_(1.0-x)Co_x alloy composition. According to literature findings no theoretical attempts have been made on ZrNbCo alloy system thus far.

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Hasani Chauke. chaukehr@ul.ac.za

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Primary author: Mr MALEBATI, Magoja Martinus (University of Limpopo)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Mr MALEBATI, Magoja Martinus (University of Limpopo)

Session Classification: Poster Session (1)

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