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## **<b>Structural and thermodynamic properties of Zr-Nb-Co</b>**

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More advanced Zr-based alloys are being developed for the more severe operating conditions such as higher burn-up and increased operation temperature, this is due to their good resistance to corrosion and high melting point. In this work, density functional theory have been used to investigate the structural and thermodynamic properties of Zr-Nb-Co system at various concentrations. We used the virtual crystal approximation to introduce small Co content on different Zr-Nb composition, Zr<sub>78</sub>Nb<sub>22</sub>, Zr<sub>97</sub>Nb<sub>3</sub>, Zr<sub>98.1</sub>Nb<sub>2</sub>, Zr<sub>99</sub>Nb<sub>1</sub>, We found that the increase in Co concentration enhances the stability of the compound with the Zr<sub>78</sub>Nb<sub>22</sub> being the most preferred composition, and the alloy is stable only at a small Co concentration of about 3%. The structure were also confirmed using XRD patterns. we also found that the Zr<sub>78</sub>Nb<sub>17</sub>Co<sub>3</sub> structure is stable above 900K

**Apply to be considered for a student award (Yes / No)?**

Yes

**Level for award (Hons, MSc, PhD, N/A)?**

MSc

**Main supervisor (name and email) and his / her institution**

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**Would you like to submit a short paper for the Conference Proceedings (Yes / No)?**

No

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