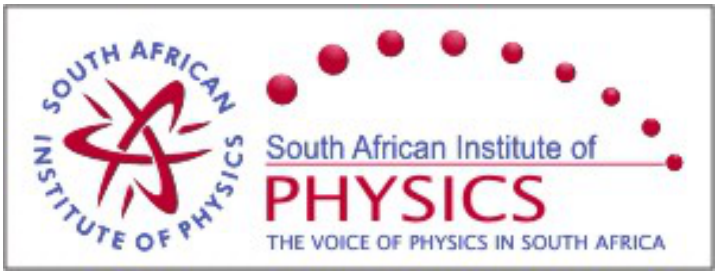

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Computational Study of the Structural and Stability of the Noble Metal Alloys X3Al (where X = Pt, Pd, Os, Ir, Rh and Ru)

We have used electronic structure method based upon Density Functional Theory (DFT) formalism to search for new class of high temperature super-alloys. Our search is focused on alloys between the noble metals and aluminum. Over-estimation of the properties of our target alloys was avoided by approximating only the gradient of the exchange and correlation functional. The behavior of each alloy to stress was investigated using volume-conserving strains. Our calculation's result predicts that alloys based on iridium (Ir) and rhodium (Rh) should combine good high temperature strength with structural stability.

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