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COMPUTATIONAL MODELLING STUDIES OF Fe-Al-X (X= Pt, Ru) ALLOYS

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Iron aluminides intermetallic compounds are regarded as promising materials for industrial applications because of their low cost, low density, high temperature strength, as well as excellent oxidation and corrosion resistance. The Fe-Al based systems have recently attracted a lot of attention as a potential replacement of steel due to their excellent resistance to oxidation at high temperatures, yet limited room temperature ductility and a sharp drop in strength above 600 oC. These intermetallic ordered structures have attracted great interest for both scientific and possible technological applications, mainly based in the stoichiometric compositions of Fe₃ Al and FeAl, have a great potential in a variety of structural application such as Stainless Steel Coatings, automobile and aero-space industry in substitution of superalloys. The study will employ Density functional theory (DFT) to investigate the ground state energies of many-body systems using MedeA (VASP) and Materials Studio (CASTEP code) in order to compute the electronic structure of materials and observing similar and distinctive characteristic and behavioural properties of these alloys at different percentages. The calculated cut-off energy of 500 eV, various number of k-points and geometry optimisation reveals the relaxation and stability behaviour of Fe-Al alloys. Density of states will further describe the interval of energy at each energy level that are available to be occupied At. 0% to 100% wherelse FeAl at. 50% has minimum number of density of states at fermi level in a phase diagram. Phonons will be shown to further elaborate that they are in agreement with the density of states obtained.

Apply to be
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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
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Yes

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