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First principle study of structural, magnetic, electronic and mechanical properties of A15 X3Ru alloys

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Ruthenium based alloys have excellent properties which makes them good candidates for high temperature applications. A large number of equipment such as turbine and spacecraft engines operates at high temperatures in aggressive chemical environments. Therefore there is a need to search for materials that can withstand extreme thermal, chemical and mechanical conditions for these applications. This study aims to develop high temperature materials with good oxidation and corrosion resistance. We discuss trends in structural, magnetic, electronic and mechanical properties of 3d transition A15 X3Ru alloys (X = Sc, Ti, V, Cr, Mn, Co, Cu, Ni, Fe and Zn) observed using First principle density functional theory calculations. The heats of formation predict an increase in stability in the following trend: Ti3Ru > V3Ru > Cr3Ru > Mn3Ru. We find that Ni3Ru, Fe3Ru, Co3Ru and Mn3Ru compounds have magnetic moments of 1.0, 1.6, 1.7 and 2.6 μB/atom. The density of states indicates that Sc3Ru, Ti3Ru, V3Ru and Cr3Ru systems are metallic due to valence-conduction overlap in the Fermi energy level, whilst X3Ru (Mn, Fe, Co and Ni) are half-metallic with 100% spin polarization at the Fermi level. Furthermore, the ratio of bulk to shear modulus indicates ductility in X3Ru (X = Sc, Ti, V, Cu, Ni, Mn, Cr and Zn) suggesting that these systems are mechanically stable. Doping the X3Ru (X = Sc, Ti, V, Cr, Mn, Co, Cu, Ni, Fe and Zn) alloys with transition metals such as Nb, Ta, Pd or Pt improves their structural, electronic and mechanical properties.

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