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Surface Segregation and Stability of PdRuM (M=Rh, Ir, Ni, Ag) Ternary Metal Alloy Surfaces Through First Principles-based Studies SUSAN ASPERA, RYAN AREVALO, HIROSHI NAKANISHI, HIDEAKI KASAI, National Institute of Technology, Akashi College — Owing to the wide variety of possible combinations and promising applications, interest in the studies on the properties and behavior of transition metal alloys have been shown from the numerous studies to date. Recent advancement in nanoparticle science shows that binary transition metal nano-alloy particle shows remarkable properties different from that of its bulk form. At this point, the possibility of unravelling more interesting properties may arise from the combination of ternary transition-metal alloys. In this study, we used density functional theory (DFT)-based calculation and analysis to determine surface segregation and stability of ternary transition metal alloys. To sample, we used the ternary PdRuM (M= Rh, Ir, Ni, Ag). Our results show that surface effects and atom-atom interaction in the binary system have large factors in the formation of ternary metal nano-particle alloy. And depending on the type of atom combination, tendency for surface segregation has drastic effects. One of the distinct properties of nano-particles are its larger surface area as compared with its bulk form. As such, this could be translated to a dominating factor for stability and behavior of nano-particle alloys.

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