First Principles Study of Surface Stability and Segregation of PdRuRh Ternary Metal Alloy System

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Highlights

- We analyzed the surface stability and segregation of ternary metal alloy system PdRuRh through first principles calculation using density functional theory (DFT) method.
- The main factors that were considered in this study are: (1) the possibility phase formation upon alloying, i.e., mixing of constituent atoms, segregation and a combination of both, and (2) the kind of surface atoms.
- Our results show that for the ternary combination of Pd, Rh and Ru, Pd atoms have the tendency to segregate at the surface, and due to the good interaction between Ru and Rh atoms, they tend to mix at the bulk of the system.
- We also determined that the trend of stability in the binary alloy system is a good determinant of stability in the ternary alloy system.
- These results are important guiding principles in the materials design of surfaces consisting of ternary metal alloy surfaces.