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Exploring enhanced titanium (Ti) nanoclusters doped with osmium (Os) and ruthenium (Ru): A DFT study

Doped transition metal nanoclusters have gained significant interest for essential scientific research and various application purposes in catalysts, electronic and biomedicine. Elemental alloying of nanoclusters is considered as an efficient way to improve their stability, electronic properties, and reactivity. However, few studies comprehensively evaluating the effects of alloying Os and Ru on Ti nanoclusters are available. In this study, structural and electronic properties of TiN-1M (N = 2-20, M = Os, Ru) nanoclusters have been investigated using density functional theory technique. The calculations showed that osmium impurity prefers to be encapsulated and ruthenium mostly prefers the apex of titanium nanoclusters. The Os and Ru impurities are observed to enhance the binding energy of pure titanium nanoclusters with Os impurity having the least binding energy. The relative stability and the dissociation energy revealed that the doping of Os and Ru enhances the stability of N = 13 nanocluster. The HOMO-LUMO gap shows the same energy gaps for Ti and Os doped Ti nanoclusters and all the impurities are observed to have a similar gap at N = 17. The is a correlation between relative stability, dissociation energy and the HOMO-LUMO at N = 13 and 17.

Keywords: Binding energy, relative stability, dissociation energy, HOMO-LUMO

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