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Insight into the effect of rhodium atom on TiN (N = 1 – 20) nanoclusters: A DFT investigation

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Doping monometallic nanoclusters with other transition metal atoms have received significant attention since they can be rationally designed and integrated to achieve unique properties and functions. These properties are suitable for use in applications such as catalysis, microelectronics and nanotechnology. In this study, a density function theory approach was employed to investigate the structural and electronic properties of TiNRh (N = 1-20) nanoclusters. The calculations showed that rhodium impurity prefers the apex and mostly occupies the faces of titanium nanoclusters. The Rh doped Ti nanoclusters revealed enhanced binding energy in comparison with bare Ti nanoclusters. The relative strength displayed the shifting of the stability from N = 7 for pure Ti nanoclusters to N = 13 for Rh doped Ti nanoclusters. Furthermore, the dissociation energy showed excellent correlation with the relative stability trend. The HOMO-LUMO revealed the lowest energy gap at Ti12Rh (N=13), which correlates well with the relative stability and dissociation energy.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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