Contribution ID: **248** Type: **Poster Presentation**

structural and electronic properties of TiNOs (N = 1-15) clusters:A density functional theory study

Doped transition metal nanoclusters have attracted significant interest for essential scientific research and various application purposes such as heterogeneous catalysts, electrochemistry and alloy designs. However, the current understanding of titanium bearing bimetallic nanoclusters is far from satisfactory. This is due to the complexity of the almost empty d band. The concept of metal doping of nanoclusters provides an opportunity to tune their activity and selectivity. In this study, structural and electronic properties of TiN-1Os (n = 2 –16) clusters have been investigated using density functional theory. The calculations showed that Osmium impurity prefers to be encapsulated and mostly occupies the face and surface of titanium nanoclusters. The Ti6Os and Ti12Os nanoclusters are found to be more stable. Interestingly, Osmium dopant converted N = 13 as the magic cluster. The HOMO-LUMO gave the lowest energy gap at Ti12Os (N = 13), which correlates well with the predicted binding energy, relative stability and dissociation energy

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

yes

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

honours

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Session Classification: Poster Session

Track Classification: Track G - Theoretical and Computational Physics