Contribution ID: **169** Type: **Poster Presentation**

Density functional theory study of Ti _n (n = 2-32) clusters: Lowest energy configurations and electronic properties.

Tuesday, 4 July 2017 17:10 (1h 50m)

The geometrical structures and electronic properties of transition metal clusters have been extensively studied during the past decades. However, theoretical investigations on titanium metal clusters have not been carried out systematically up to the larger clusters. In this study, density function theory (DFT) calculations have been performed to investigate the lowest energy structures and electronic properties of Ti_n (n = 2-32) clusters using PBE-Sol spin-unpolarized exchange correlation functional. Most of the previous studies revealed the distorted icosahedral and pentagonal bipyramid geometry as the most stable clusters among the other clusters. Nevertheless, this study predicted that Ti clusters follow the pentagonal behaviour. Triangular bi-pyramid Ti₅ with (D_{3h}) symmetry and pentagonal bi-pyramid Ti₇ with (D_{5h}) symmetry were found to be the most stable clusters compared to their neighbours.

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

Yes

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

MSc

Main supervisor (name and email)
and his / her institution

Prof H. R Chauke
Hr.Chauke@ul.ac.za
University of Limpopo

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Mr PHAAHLA, Tshegofatso Michael (University of Limpopo)

Presenter: Mr PHAAHLA, Tshegofatso Michael (University of Limpopo)

Session Classification: Poster Session 1

Track Classification: Track A - Division for Physics of Condensed Matter and Materials