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

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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_{5h}) symmetry and pentagonal bi-pyramid Ti₇ with (D_{5h}) symmetry were found to be the most stable clusters compared to their neighbours.

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Level for award

dr> (Hons, MSc,

%nbsp; PhD, N/A)?

MSc

Main supervisor (name and email)

sand his / her institution

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Yes

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