Structural Evolution and Electronic Properties of Intermediate Sized Ti_n (n=33--60) Clusters

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Abstract

The structural evolution of Ti_n ((Formula presented.)) clusters has been investigated by using the systematic cluster growth method together with the many-body Gupta potential. The lowest energy structures are further refined by using density functional theory computations within the accuracy of the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional and a plane-wave basis set. Using this approach, the structures and stability trends of Ti_n clusters in the (Formula presented.) size range previously reported, are reproduced. New clusters with enhanced stability are found for (Formula presented.), 38, 41, 43, 46, 48, 50, 53, 55, and 58 sizes. Tightly packed structures dominate principally for these clusters in which the shape of the structures can be understood based on the encapsulated motif. The geometries of the clusters from Ti_{33} up to Ti_{60} adopt oblate forms which is in contrast to the smaller clusters. The vertical ionization potential (vIP) and vertical electron affinity (vEA) curves show a step behavior depending of the size range for (Formula presented.), while the chemical hardness decreases monotonically with the size, which is consistent with the d-band center parameter. In contrast to previous reports, for (Formula presented.) it is found that a distorted Mackay icosahedron is more stable than the regular one. The theoretical electronic properties for the most stable isomers of Ti_n clusters are in good agreement with the available experimental data. © 2021 Wiley-VCH GmbH

Author keywords

clusters; density functional theory; structure; titanium