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Structural evolution, growth and stability of metal titanium clusters. HASANI CHAUKE, TSHEGOFATSO PHAAHLA, PHUTI NGOEPE, Materials Modelling Centre, University of Limpopo, Department of Physics, Private Bag x1106,Sovenga., RICHARD CATLOW, Centre for Material Research, University College London, Department of Chemistry, Gower Street, London, WC1E6BT — The transition metals clusters such as titanium have received a significant attention due to their excellent physical and chemical properties and great technological application in many fields. A survey of small Ti clusters was performed using interatomic potentials and computational methods based on density functional theory; and the knowledge led master code with a genetic algorithm to generate the lowest energy geometries of Tin (n = 2-32) clusters. The all electron spin-unpolarized generalized gradient approximation is used to determine the ground state structures, binding energy and electronic properties. The structural evolution of titanium clusters, which favors the icosahedron structure growth pattern is observed. The energy for the ground state configurations is found to increase monotonically with the clusters size. Their relative stability results predict clusters with 5 and 7 as more stable. The energy difference for clusters n$\geq$24 is very small, suggesting that the larger clusters could be stable at moderate temperatures. In addition to the magic numbers that are often reported i.e. Ti7 and Ti13; clusters 5, 9, 14, 17 and 26 have extra stability.

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