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Geometry and Electronic Properties of TinPt (n = 2–7) Clusters: A Density Functional Theory Study

Thursday, 11 July 2019 15:00 (2 hours)

Nanoscale clusters are considered a new phase of matter, being the bridge between atoms and the bulk. They form part of extensive research due to their various potential applications. There is considerable interest in the structures and properties of nanoscale clusters, for example, being used as finely divided metal catalysts, particularly for bimetallic clusters, which offer the opportunity of tuning their activity and selectivity. To date, much work has been concentrated on small clusters of late transition metals™, namely, noble and platinum metals, while little has been done for the early transition metals. Among TM clusters, the reactivity of titanium clusters is not fully understood due to the complexity of the almost empty d band, which provides unique bonding properties. In this study, we investigate the structures and electronic properties of TinPt (n = 2–7) clusters using density functional theory with the generalized gradient approximations (PBEsol and PBEsol0). The stability of the clusters is also studied whereby the consistency of TinPt (n = 2-7) clusters with pure Tin (n = 2-7) clusters is considered. PBEsol was found to be overestimating the energies of the clusters.

Apply to be
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Yes

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

PhD

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