Evolution of small Ti clusters and the dissociative chemisorption of $\text{H}_2$\textsuperscript{1} T.J. DHILIP KUMAR, P.F. WECK, Department of Chemistry, University of Nevada Las Vegas, B. NADUVALATH, Department of Chemistry, University of Nevada Las Vegas, 4505 Maryland Parkway — The addition of small Ti clusters in certain complex metal hydrides has been found to improve significantly the kinetics of $\text{H}_2$ adsorption and desorption processes. The catalytic activity of doped Ti in these hydrogen storage materials is not fully understood. Here we report a systematic study of the sequential growth of small Ti clusters from $n = 2 - 15$ atoms and the dissociative chemisorption of $\text{H}_2$ on the minimum energy clusters using density functional theory under the generalized gradient approximation. It has been found that the low energy clusters follow a pentagonal growth pattern. The clusters Ti$_7$ and Ti$_{13}$ show higher stability with a configuration of pentagonal bipyramid and icosahedron structures, respectively. The second difference of binding energy plot indicates that these two clusters are highly stable which agrees with the experimental collision-induced dissociation studies. Subsequently, a systematic study of the chemical reactivity of small Ti$_n$ clusters with $n = 2 - 15$ towards dissociative chemisorption of $\text{H}_2$ has been performed. It is found that the chemisorption occurs preferentially at the two adjacent edges of any Ti atom. The chemisorption energy as a function of cluster size shows considerable structural changes in the Ti$_n$ clusters due to $\text{H}_2$ adsorption and dissociation.

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