Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Evolution of small Ti clusters and the dissociative chemisorption of H_2[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 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 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 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 H_2 adsorption and dissociation.

[1]This work is supported by DOE Grant DE-FG36-05GO85028.

Balakrishnan Naduvalath
Department of Chemistry, University of Nevada Las Vegas

Date submitted: 26 Nov 2006 Electronic form version 1.4