PAPER ID:91

A DFT STUDY OF Ti-DOPED Al NANOCLUSTERS FOR HYDROGEN BASED TRANSPORT VEHICLES

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ABSTRACT

Hydrogen has shown its potential for cleanand sustainable fuel for future transport vehicles. However, safe, efficient, and economical production & storage of the hydrogen still remains a bottleneck for the hydrogen vehicle technologies [1,2]. Additionally, aluminum is a cheap metal that has the capability to store hydrogen using its adsorption kinetics [3]. The high surface to volume ratio of the nano-clusters is a desirable property for surface phenomenon such as adsorption [4]. Experimental studies have shown that Al nano-clusters are stable and therefore are lucrative hydrogen storage materials [5,6]. Extensive efforts have been made to increase the hydrogen binding to Al clusters by suitable doping [6–10]. Nevertheless, the effect of Ti doping in Al clusters still remains obscure. Therefore, the present study aims to investigate the effect of Ti doping on stability and site preference in Ti doped Al_5clusters. Further, the interaction of the ground state $TiAl_4$ cluster with molecular hydrogen has also been investigated. To predict the Ti-doped structures and the properties of Ti-Al nano-clusters, Density Functional Theory (DFT) is employed as implemented in the Vienna abinitio simulation package (VASP) using general gradient approximations (GGA) without imposing any symmetry constraints. The study shows that the Al_5 cluster exists in two stable ground state geometric configurations with planar W shape and square pyramidal C_2V symmetry. The Ti-doped cluster is more stable than the bare Al_5 nano-clusters. The Ti atom prefers the site which has maximum Ti-Al bonds. The Ti-Al bond length is small as compared to the Al-Al bond length resulting in slight geometric distortions in the Al clusters. Hydrogen interaction study shows that hydrogen adsorption energy on the $TiAl_4$ cluster is as low as -0.026 eV/ atom. Thus, Ti-Al nano-clusters are a stable, efficient and economical candidate for hydrogen storage materials.

Keywords: Hydrogen Storage, Al nano-clusters, Alternative energy source, Density Functional Theory