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Adsorption and dissociation of H_2 on Pd doped graphene-like SiC sheet

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ABSTRACT

Doped porous SiC nanostructures with metallic atoms, nanoclusters and nanoparticles have been recognized as promising materials for hydrogen storage. With this regards transition metal elements are interesting impurities for use as doping. In view of this prospect, a theoretical approach based on density functional theory (DFT) was applied to study of the interaction between hydrogen molecule and a graphene-like SiC sheet doped with palladium atom. We have selected a single graphene-like SiC layer, due to its more surface charge polarization in comparison with pure graphene which makes possible remarkable interactions with adsorbed hydrogen molecules. In our study we have included two different configurations of H_2 adsorption: 1) at the first state, hydrogen atoms after adsorption stretched and distance between H–H atoms has increased but their chemical bond doesn't break. In this situation a physical adsorption occurred and the binding energy restricts applicable interests where it is appropriate for reversible hydrogen storage; 2) at the second situation, atoms of hydrogen molecule discrete from each other and adsorption occurred in a chemical manner. As instance the when a H_2 molecule interact simultaneously with Pd atom and SiC nanosheet, it can be dissociated as in this case a hydrogen atom makes bond with Pd atom and the other can be adsorbed chemically on the SiC nanosheet surface. More details about adsorption mechanism are discussed it the context.

Introduction

Fuels based on hydrogen storage capability are systems that release very little environmental pollutants unlike fossil fuels. The use of hydrogen-based fuel cells needs solutions for the current challenges in the realm of technology. For instance we can point out to synthesize and design of the advance materials to reduce the costs of the hydrogen generation, transmission and maintenance [1]. Nanotechnology has introduced new materials with vast range of applications. Among them, carbon nanotubes, fullerenes, and graphene are extremely noteworthy. Recently, graphene-based materials included many significant researches, especially in the field of catalysis, electronics, optics and electro-chemical oxidation

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