Coupled Systems Mechanics, *Vol. 3, No. 4 (2014) 329-344*
DOI: http://dx.doi.org/10.12989/csm.2014.3.4.329

Molecular dynamics studies of interaction between hydrogenand carbon nano-carriers

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(Received March 1, 2013, Revised April 8, 2013, Accepted May 5, 2013)

Abstract. In this work, quantum molecular dynamics simulations (QMD) are preformed to study the hydrogen molecules in three types of carbon nanostructures, C_{60} fullerene, (5,5) and (9,0) carbon nanotubes and graphene layers. Interactions between hydrogen and the nanostructures is of importance to understand hydrogen storage for the development of hydrogen economy. The QMD method overcomes the difficulties with empirical interatomic potentials to model the interaction among hydrogen and carbon atoms in the confined geometry. In QMD, the interatomic forces are calculated by solving the Schrodinger's equation with the density functional theory (DFT) formulation, and the positions of the atomic nucleus are calculated with the Newton's second law in accordance with the Born-Oppenheimer approximation. It is found that the number of hydrogen atoms that is less than 58 can be stored in the C_{60} fullerene. With larger carbon fullerenes, more hydrogen may be stored. For hydrogen molecules passing though the fullerene, a particular orientation is required to obtain least energy barrier. For carbon nanotubes and graphene, adsorption may adhere hydrogen atoms to carbon atoms. In addition, hydrogen molecules can also be stored inside the nanotubes or between the adjacent layers in graphite, multi-layer graphene.

Keywords: quantum molecular dynamics simulation; hydrogen; carbon; fullerene; nanotube; graphene

1. Introduction

The hydrogen storage problem is critical for the development of hydrogen economy (Strobel *et al.* 2006). In fact, the science about hydrogen, even though a very old subject, still requires detailed studies in terms of its behavior under high pressure (Labet *et al.* 2012). In addition to using metal hydrides, or other methods, such as methane carbon dioxide reforming (Ni 2013), nano-cages provide an ideal solution to be a hydrogen carrier. Using carbon carriers for hydrogen storage has been studied by the *ab initio* simulation method (Dodziuki 2005, Ding *et al*. 2007, Pupysheva *et al*. 2008, Lin *et al*. 2008, Singh *et al*. 2009, Kruse *et al*. 2009), as well as experimental methods (Lachawiec *et al*. 2005, Lee and McKee 2008, Stadie *et al*. 2010). In addition to fullerenes, using carbon foam for storing hydrogen by physisorption and chemisorption is reported (Ding *et al.* 2007). For larger nanostructures, or called nanocages, molecules which are formed as a metal organic framework is an plausible candidate (Er *et al.* 2009). To improve the simulation accuracy, efforts have been placed to consider the non-covalent interaction in the hydrogen-carbon system (Kruse *et al.* 2009). By combining experimental and computational

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http://www.techno-press.org/?journal=csm&subpage=7 ISSN: 2234-2184 (Print), 2234-2192 (Online)

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