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Hydrogen storage on silicon, carbon, and silicon carbide nanotubes: A combined quantum mechanics and grand canonical Monte Carlo simulation study

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ABSTRACT

Grand canonical Monte Carlo (GCMC) simulation combined with ab initio quantum mechanics calculations were employed to study hydrogen storage in homogeneous armchair open-ended single walled silicon nanotubes (SWSiNTs), single walled carbon nanotubes (SWCNTs), and single walled silicon carbide nanotubes (SWSiCNTs) in triangular arrays. Two different groups of nanotubes were studied: the first were (12,12) SiNTs, (19,19) CNTs, and (15,15) SiCNTs and the second were (7,7) SiNTs, (11,11) CNTs, and (9,9) SiCNTs with the diameters of ~ 26 and ~ 15 Å for the first and second groups, respectively. The simulations were carried out for different thermodynamic states. The potential energy functions (PEFs) were calculated using ab initio quantum mechanics and then fitted with (12,6) Lennard-Jones (LJ) potential model as a bridge between first principles calculations and GCMC simulations. The absolute, excess, and delivery adsorption isotherms of hydrogen were calculated for two groups of nanotubes. The isosteric heat of adsorption and the radial distribution functions (RDFs) for the adsorbed molecules on different nanotubes were also computed. Different isotherms were fitted with the simulation adsorption data and the model parameters were correlated. According to the results, the hydrogen uptake values in (19,19) CNT array exceeded the US DOE (Department of Energy) target of 6.0 wt% (FY 2010) at 77 K and 1.0 and 2.0 MPa for absolute and excess uptakes, respectively. The results also show that SiNTs and SiCNTs are not more useful materials compared with corresponding CNTs for hydrogen storage.

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1. Introduction

It is estimated that the world energy consumption will double over the current half century [1]. Meeting this demand while maintaining or reducing our current environmental footprint

will require significant changes in the way we produce, distribute, store and use energy. On one hand, the development of social economy and culture brings many of us high standards of living; on the other hand, our world is facing a rapid depletion of natural resources and serious global environmental problems. A crucial step in this process is

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reducing our dependence on carbon-based fossil fuels and developing alternatives that are environmentally friendly and renewable [2].

Hydrogen is an ideal candidate as it is available from domestic renewable resources, and usable without pollution. Some of its advantages are: environmentally compatible, easy to produce, highest heating value per mass of all chemical fuels, convenient fuel for transportation, versatile, converts easily to other energy forms at the user end, and high utilization efficiency [3–5]. Therefore, hydrogen provides the best route to a sustainable energy for the transportation sector and some other uses, since it can be produced not only from the fossil fuels, such as coal and natural gas, but also from wind, solar, thermal, hydroelectric, biomass or municipal solid wastes with no consumption of non-renewable resources and no pollution of any kind. Until now, full implementation of a hydrogen-based energy system has been hindered mainly by the challenge of storing hydrogen gas, both on-board (reversible) and off-board (non-reversible) applications [6].

Hydrogen can be traditionally stored using five different methods and phenomena [7]: (1) high-pressure gas cylinders (up to 800 bar), (2) liquid hydrogen in cryogenic tanks (at 21 K), (3) trapping on interstitial sites in a host metal (at ambient pressure and temperature), (4) chemically bonded in covalent and ionic compounds (at ambient pressure), and (5) through oxidation of reactive metals, e.g. Li, Na, Mg, Al, Zn with water. All of these methods have one or more disadvantages like unsafe issues (very high pressure of storage), low storage efficiency (due to low critical temperature of hydrogen of 33 K), high material and storage cost (bulky and heavy steel tanks, expensive reactants, and providing very low storage temperatures), hazardous side products (especially for oxidation approach), large amount of energy is needed (liquid hydrogen), and non-reproducibility or irreversibility.

A number of novel storage techniques have been investigated to complement the currently available methods where hydrogen is stored in gaseous [8]. Physical adsorption (physisorption), particularly using microporous materials, has earned considerable attention for its safe nature and the potential for a high storage density of hydrogen in order to reach to US DOE (Department of Energy) target of 6.0 wt% by the FY 2010, and 9.0 wt% by the FY 2015 [9]. The most important micropore materials for hydrogen storage processes considered yet include zeolites [10], activated carbon and carbon molecular sieves [11,12], coordination polymers [13], metal organic frameworks (MOFs) [14], and covalent organic frameworks (COFs) [15].

One of the major problems is the difficulty of finding efficient adsorbents. Nanotubes are one of the convenient candidates for hydrogen storage due to their large specific surface area and numerous adsorption sites at which gases can react with. Many efforts have been conducted both experimentally and theoretically to explore such this possibility [16–19]. However, most of the experimental and theoretical efforts in this area so far have failed to approach the proposed target. In addition, their results are sometimes controversial and cannot be applied practically.

Since discovery of carbon nanotubes by Iijima [20], these materials have been used as a promising candidate in

various applications [21]. Especially gas adsorption on single walled carbon nanotubes (SWCNTs) is a subject of growing experimental and theoretical interest [22]. Light and medium weight hydrocarbons [23–25], nitrogen [26], neon [27], helium [28], xenon [29], and ammonia [30] are some examples of materials that their physisorption on CNTs were studied till now.

Silicon is often suggested as a substitute for carbon because of its chemical similarity but some differences exist between C and Si bonding characteristics [31]. One of the interesting silicon based nanostructures is the silicon nanotubes (SiNTs) which is similar to the CNTs [32,33]. The existence of SiNTs has been proved by theoretical methods such as density functional theory (DFT) [34–39], Hartree-Fock [37–39], Møller–Plesset electron correlation [38], and semi-empirical [37]. A variety of experiments have been applied to synthesis the pure SiNTs [40]. In the recent years, SiNTs have been considered as a promising candidate for gas adsorption and separation [18,41–43].

In 1999, the production of heterofullerenes containing Si up to 50% was achieved [44] and in 2001 the first synthesis of silicon carbide nanotubes (SiCNTs) was reported [45]. The SiCNTs containing only Si–C bonds are more stable than those contain C–C and/or Si–Si bonds [46] for this reason we selected this type of SiCNTs for the present work. There are several publications which focused on adsorption of different gases such as H₂, N₂, CO₂, NO₂, C₄H₁₀, NH₃, and HCOH on SiCNTs [17,19,47–50].

Various strategies have been applied to prepare various nanotubes with high yield, low cost, and high purity. These processing routes include: arc-discharge, laser evaporation, and chemical vapor deposition. Some large-scale and low-cost techniques have been employed for production of CNTs such as catalytic pyrolysis of benzene at 1200 °C [51], catalytic decomposition of ethylene at 800 °C [52], catalytic decomposition of light and medium alcohols by a novel aerosol method [53], catalytic pyrolysis of CCl₄ using supercritical carbon dioxide as a medium at 175 °C [54]. A variety of methods have been applied to produce large scale SiNTs and SiCNTs with high quality and a reasonable cost [40,55–57]. The structural, thermal, and electrochemical stability of these nanotubes have been proved theoretically and experimentally [46,58,59].

The aim of the present work is to explore hydrogen physisorption on SWSiNT, SWCNT, and SWSiCNT triangular arrays by employing the multiscale theoretical study which combines ab initio quantum mechanics calculations and grand canonical Monte Carlo (GCMC) simulation. Two different NT groups all with armchair configuration, were considered: the first were (12,12) SiNTs, (19,19) CNTs, and (15,15) SiCNTs and the second were (7,7) SiNTs, (11,11) CNTs, and (9,9) SiCNTs with the diameters of 26 and 15 Å for the first and second groups, respectively. The armchair configuration was chosen because of its more stability compared with zigzag configuration [35,46,60]. The simulations were carried out at different thermodynamic conditions. The PEFs were calculated using ab initio quantum mechanics and then fitted with (12,6) LJ potential model as a bridge between first principles calculations and GCMC simulation.

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