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A Combined Computational and QM/MM Molecular Dynamics Study on Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) as Hydrogen Storage

A Heidari

Faculty of Chemistry, California South University, CA, USA

Corresponding author: A Heidari

Scholar.Researcher.Scientist@gmail.com

Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA.

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Environmental concerns regarding the use of fossil fuels and their predicted exhaustion are globally important issues. Currently, the commercially available Hydrogen storage method is interesting. The Faculty of Chemistry of California South University (CSU) is the sponsor for these researches and has announced 12.0% wt storage for solid–state on–board systems; target of the Faculty of Chemistry of California South University (CSU) is found materials with this capacity and reversible mechanism for these systems. Although the storage mechanism is not completely clear yet, there is a big argument in chemical and physical adsorption on the surface of materials. Therefore, materials with high specific surface area are suitable. Materials for Hydrogen storage can be category in two huge groups, Carbon base materials specially Carbon Nano Tubes (CNTs) and non–Carbon base materials such as metal hydrides, chemical hydrides, alloys in nano crystal forms and non–Carbon nanotubes (N–NT) [1–11].

In addition, Carbon nanotubes (CNTs) have diverse applications from nano–electronics to nano–biotechnology and show unique properties but because of diameter and chirality dependence of the properties, non–Carbon nanotubes (N–NT) independent of determining factors, e.g., Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) which are always semi–conductor, became very interesting for researchers. In comparison, Carbon nanotubes (CNTs) have equivalent tubular surface; however, in tubular surface of Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs), Boron atoms relax inward and Nitrogen atoms relax outward of the surface. In other words, Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) have two different terminating atoms of Boron and Nitrogen. In this editorial, a new idea about Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h– BNNTs) is considered. Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) have different terminating atoms; however, in the current editoial, the electronic structure of Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) models consisting of two Boron terminating atoms is studied. The computations are done by Gaussian 09 and at the level of DFT methods.

Also, Carbon nanotubes (CNTs) offer unique electrical properties such as the highest current density, which are three orders of magnitude higher than Copper, ultra–high thermal conductivity as high as that of diamond. Meanwhile, Hydrogen is an ideal fuel; it is abundant, renewable, and its combustion produces only water vapor and heat, is efficient and safe and it will play an important role in the future world energy structure. In this editorial, Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) of various sizes such as zigzag (6, 0), zigzag (10, 0), armchair (6,6) and armchair (10, 10) optimized by HF, HF+MP2, LDA, BLYP, B3LYP, MP2, MP3 and MP4 methods using 6–311++G (d, p) basis set of the Gaussian 09 and after first optimization, was added Hydrogen molecules in to the nanotubes, then in each level increased amount of Hydrogen molecules in to the nanotubes. By computations the vacant volume of the nanotubes was measured and added Hydrogen molecules to this volume in several steps until to complete this space. The current editorial had been more attention to amount of stability and interaction between nanotubes and Hydrogen gas

and the aim of this editorial was that the nanotubes have been using as Hydrogen storage.

Furthermore, in the present editorial, (8, 8) close–ended Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) with 7/57 ring arrangement has been studied. Conformational and geometrical parameters of included rings in these nanotubes have been investigated by HF, HF+MP2, LDA, BLYP, B3LYP, MP2, MP3 and MP4 methods using 6–311++G (d, p) basis set of the Gaussian 09. We have also analyzed the aromaticity of these compounds by means of Nucleus Independent Chemical Shift (NICS) criterion. We have computed the Nucleus Independent Chemical Shift (NICS) values using the HF, HF+MP2, LDA, BLYP, B3LYP, MP2, MP3 and MP4 methods with 6–311++G (d, p) basis set of the Gaussian 09 for compound these structures at the a, b and c points and included rings in these compounds.

Moreover, we presented systematic molecular dynamics (MD) simulations studies of Hydrogen storage in Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs). Assuming the simple physical adsorption of Hydrogen to the surfaces of Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs), potential forms between H_2–H_2, N–H_2 and B–H_2 were both expressed by Lennard–Jones, Morse and Morse/Long–range potential functions. Fixing the relative coordinates of Boron and Nitrogen atoms to the center of mass of each Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs), the center of mass motion was modeled with the van der Waals force between Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs), separately. While the amount of Hydrogen adsorption per unit Boron and Nitrogen masses inside Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) increased with increasing diameter, adsorption between tubes was almost constant. The simulation studies of Hydrogen adsorption in three types of ideal Y–junction Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) with open ends were carried out using molecular dynamics (MD) simulations and molecular mechanics calculations. The results show that the physisorption of Hydrogen in Y– junction Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) are very limited and far from the target set by the Faculty of Chemistry of California South University (CSU) for Hydrogen storage and transportation, implying that it is unlikely to achieve high Hydrogen storage in open–ended–junction Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs) via physisorption scheme.

Finally, in this editorial, the effect of different values for the ε and σ parameters in the Lenard–Jones potential equation, Morse potential equation and Morse/Long–range potential equation presented for the Hydrogen gas storage on Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h– BNNTs) was studied at 110 (K) temperature and 200 (atm) pressure. The results show that a significant change does not appear in the Hydrogen density distribution by varying the potential equations. Therefore, in simulation of Hydrogen adsorption on Boron Nitride Nanotubes (BNNTs), Amorphous Boron Nitride Nanotubes (a–BNNTs) and Hexagonal Boron Nitride Nanotubes (h–BNNTs), we are easily able to thoroughly study the phenomenon of adsorption at different temperatures and pressures and also gas mixtures, due to independence of adsorption from the potential equations.

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