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# Theoretical comparative study on hydrogen storage of $BC_3$ and carbon nanotubes

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**Abstract.** We have applied the grand canonical Monte Carlo method (GCMC) to investigate the physisorption properties of hydrogen storage in $BC_3$ and carbon nanotubes, respectively. Some important physical amounts under different temperatures and pressures, such as adsorption isotherms and adsorption amounts were studied. The results show that, the physisorption properties of $BC_3$ nanotube are superior to those of carbon nanotube at all conditions. The main reasons causing such different results between them were analyzed from the interaction energies among nanotubes and $H_2$ molecules.

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**Key words**: $BC_3$ nanotube, hydrogen storage, grand canonical Monte Carlo method (GCMC)

## 1 Introduction

Hydrogen energy is a reproducible and clean energy source, which has attracted extensive attentions in recent years. The efficient storage of hydrogen is significant for its utilization as the future energy carrier; however, it is also the bottleneck for the development of hydrogen energy. The main reason is that the amounts of hydrogen stored are not satisfied with the requirement of the development of hydrogen energy [1-3]. Therefore, some researchers are still exploring new hydrogen storage materials.

Since the discovery of carbon nanotubes (CNTs) by Iijima in 1991[4], a large number of experimental and theoretical studies have been devoted in order to explore hydrogen storage of CNTs due to its large specific area and tubular structure[5,6]. However, data on the hydrogen storage capacity of CNTs are still in dispute because some experiments

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are not reproducible. The current point is that the hydrogen storage capacity of CNTs is small at room temperatures and moderate pressures and that CNTs are not superior to other carbon nanostructures for hydrogen storage[7]. The discovery of CNTs sets off a tremendous explosion for obtaining novel one-dimensional nanostructures [4]. Shortly, some new nanotubes originating from hexagonal compounds, such as $BC_3$ and BN [5,6], have been proposed. Their geometries, electronic properties and possibilities for technical applications have been investigated theoretically [8,9]. However, to our knowledge, the hydrogen storage in $BC_3$ nanotube is an open question. Therefore, we investigated the hydrogen adsorption in this nanotube using density functional theory (DFT) recently [10], and the physisorption of molecular hydrogen in $BC_3$ nanotube including both external and internal adsorption sites was compared with CNTs. The studied results show that $BC_3$ nanotube may be a better candidate for hydrogen storage than CNTs.

Based on this, the physisorption process of $H_2$ in $BC_3$ nanotube in different temperatures and pressures is investigated quantitatively using grand canonical Monte Carlo (GCMC) method. Some important physical amounts, such as adsorption isotherms under different conditions and the total interaction energies of $BC_3$(8,0)/C(8,0) nanotube and $H_2$ molecules were studied in this paper. The GCMC simulations show that the physisorption amounts of $H_2$ in $BC_3$ nanotube are superior to those of CNTs. Some reasonable explainations causing different behavior of hydrogen storage in these two nanotubes are given. These results may help experimental explorations of new possible hydrogen storage materials.

## 2 Grand canonical Monte Carlo (GCMC) method

For the hydrogen adsorption on $BC_3$ and carbon nanotubes, we have used compass force field. It is the ab initio forcefield that enables accurate and simultaneous prediction of structural, conformational, vibrational, and thermophysical properties for a broad range of molecules in isolation and in condensed phases, and under a wide range of conditions of temperature and pressure[11]. Because the nanotube host has been treated as a rigid structure, with fixed atom positions obtained from the minimized structure, only the non-bond interaction energy is calculated for hydrogen adsorption. The total host-guest interaction energy consists of the sum of a long-rang coulombic term and a short-range van der Waals (vdW) term

$$E_{total} = E_{cou} + E_{vdW}, \tag{1}$$

$$E_{cou} = \sum_i \sum_{j>1} \frac{q_i q_j}{r_{ij}}, \tag{2}$$

where $q_i$ and $q_j$ are the net atomic charges of the $i$th and $j$th atoms, respectively, and $r_{ij}$ is the distance between the $i$th and $j$th atoms. Since the electrostatic interaction is long-range interaction and the model systems are periodic, Ewald sums are used for $E_{cou}$. The