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Lithium absorption on single-walled boron nitride, aluminum nitride, silicon carbide and carbon nanotubes: A first-principles study

M. Darvish Ganji [a,*], Z. Dalirandeh [b], M. Khorasani [c]

[a] Department of Nanochemistry, Faculty of Pharmaceutical Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran-Iran (IAUPS), Iran
[b] Young Researchers and Elite club, Central Tehran Branch, Islamic Azad University, Tehran, Iran
[c] Department of Mechanical Engineering, Semnan Branch, Islamic Azad University, Semnan, Iran

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ABSTRACT

Using the DFT-B3LYP calculations we investigate the adsorption of Li atom on CNT, BNNT, AlNNT and SiCNT. We found that Li atom can be chemisorbed on zig-zag SiCNT with binding energy of −2.358 eV and charge transfer of 0.842 |e|, which are larger than the results of other nanotubes. The binding energy of Li on SiCNT is foun to be stronger than activation energy barrier indicating that Li metal could be well dispersed on SiCNTs. Furthermore, the average voltage caused by the lithium adsorption on SiCNT demonstrated that SiCNTs could exhibit as a stable anode similar to the lithium metal anode. The binding nature has been rationalized by analyzing the electronic structures. Our findings demonstrate that Li-BNNT, Li-SiCNT and Li-AlNNT systems exhibit spin polarized behaviors and can fascinating potential application in future spintronics. Also, Li-SiCNT system with rather small band gap might be a promising material for optical applications and active molecule in its environment.

1. Introduction

Lithium ions batteries (LIBs) have been widely studied due to their numerous technological applications in engineering. They are some of the most energetic rechargeable batteries available for electric vehicles, hybrid electric vehicles, and portable electronic devices such as laptops, cell phone and iPods. The electrodes of LIBs made from carbon and light weight Li. Generally, LIBs are much lighter than other types of rechargeable batteries of the same size [1,2]. Li is one of the most reactive elements, which means that a lot of energy can be stored in its atomic bonds. Therefore, LIBs are very attractive energy sources and carriers because of their high energy density and light weight. Lithium-graphite intercalation compound (Li-GIC) has been widely used as the negative electrode in LIBs [3–5]. Carbon nanotubes (CNT) and graphene are some of the most promising materials to replace the Li-GIC negative electrode. The lithium ions storage capacity of CNTs was found to be 500 mAh/g (in the form of LiC_2) [6], which is higher than the capacity of graphite (372 mAh/g) [6,7]. Experimental investigations have shown that the maximum lithium capacity of CNTs can be increased to as high as 1000 mAh/g, corresponding to the stoichiometry of LiC_3 by ball milling [8] or chemical etching [9]. CNTs can adsorb Li ions both on the outside and on the inside surfaces through the created defects or the open-ends of nanotube [8,9]. Nishidate et al. [10] studied the adsorption of Li ions on pristine single walled CNTs (SWCNTs) and defective SWCNTs using the density functional theory (DFT) calculations. They calculated the formation energies of the $n=7$, 8, and 9 defective rings and examined their stable geometries. They also estimated the Li binding energies for these defective rings and found that the binding energy of a Li atom on the defective SWCNTs is much higher than that on the pristine SWCNTs. The higher binding energy indicated that Li adsorption capability of defective SWCNTs is better than that of pristine SWCNTs. Graphene, with Li ions storage capacity of about 784 mAh/g, has much higher capacity than the graphite one [7]. Ganji et al. [11] have investigated the adsorption of Li atoms on graphene and periodic graphene nanobuds (PGNBs) by means of the DFT calculations. They found that the Li atom storage capability of PGNB can be considerably improved in comparison with the graphene monolayer, because of the present of nonagon ring (defective site) in the PGNB. Nanotubes are considered to possess special properties compared with the corresponding bulk materials because of the quantum confinement effect. Improving the adsorption performance of the pristine nanotube by modification their structure is expensive, and therefore, finding pristine nanotubes with excellent sensitivity is a highly scientific interest. CNTs are nanometer-scaled one-dimensional tubes of graphitic carbon. SWCNTs were discovered by Iijima and Ichihashi [12] and Bethune et al. [13] in 1993. The current CNT synthesis methods are arc-discharge, laser ablation, and

* Corresponding author.
E-mail address: ganji_md@yahoo.com (M. Darvish Ganji).

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chemical vapour deposition (CVD) [14,15]. CNTs have attracted widespread interest in many fields of science and technology, such as field electron emission technologies, nanoelectronics, composite materials, switches, nanobiotechnology, artificial muscles, battery devices, and sensors, etc [16–19] due to their diverse exceptional properties including uniform porosity, high tensile strength, structural stability and high conductivity [14,20–28].

Following the syntheses of CNTs, the nanotubes of another hexagonal compound, BN, were theoretically predicted by Rubio et al. in 1994 [29,30] and then Chorpa et al. [30,31] synthesized the pure BNNTs for the first time in 1995. BNNTs made of BN honeycomb layers using various methods [32–34]. BNNTs, isosteres of CNTs, have attracted much research attention because of their unique properties such as high thermal conductivity, strong hardness, chemical inertness, and mechanical strength [29,35–41]. Elements of group III nitride nanotubes, e.g. BN and AlN are semiconductors with a wide band gap whose electrical properties are independent of diameter, chirality, and the number of the walls of the tube, and among them, AlNNT has the largest optical band gap [29,32,37,42]. All these factors prompted us to investigate the properties of BNNTs in Li adsorption. AlNNTs of a wide range of diameters (up to 80 nm) were recently successfully synthesized by different research groups [43,44]. Recently, many studies have been devoted to AlNNTs because of their good physical, chemical properties such as enhanced field emission, high thermal conductivity, large electrical resistivity, and electrostatic forces between Al and N nucleuses [45,46]. These properties make them excellent candidates for sensors, actuators, optoelectronic devices and nano-electromechanical systems [47,48].

On the other hand, silicon carbide nanotubes (SiCNTs) have been synthesized with a Si to C ratio of 1:1 via the reaction of Si with CNTs [49]. Theoretical studies of single-walled SiCNTs (SWSiCNTs) have shown that the energetically favorable structure consists of alternating Si and C atoms with each Si (C) atom having only C (Si) atoms as their nearest neighbors [50,51]. SiCNTs may possess high reactivity of exterior surface facilitating to sidewall decoration and stability against oxidation in air at high temperatures [49,52–54], which may have several interesting applications in nanoelectronics. Mpourmpakis et al. [55] have investigated the adsorption of H atoms on SiCNTs and CNTs. They reported that the binding energy of the H atom on the SiCNT is higher than that on the pure CNT due to the alternative charges existing on the SiCNT wall. The obtained results show that the alternative charges on the adsorbents surfaces can enhance its adsorption capacity.

In this work, we carry out a detailed study of interaction between four types of nanotubes (CNT, BNNT, AlNNT and SiCNT (Fig. 1)) and Li atom by using the state-of-the-art DFT-B3LYP calculations. The computational details for calculating the binding energies and the method of construction of Li/nanotubes complexes are given in detail in the next section.

2. Computational methods

Before the doping of Li atom, the 1D structure of nanotubes were first constructed and optimized according to the well-known cluster model. Indeed, the unit cells of the 1D nanotubes are very large, which make it impractical to investigate nanotubes with the first-principles calculations. Therefore, we adopt here the generally employed cluster model method to simulate the real structure of nanotubes for reducing computational cost.

All the *first-principles* calculations were performed by means of

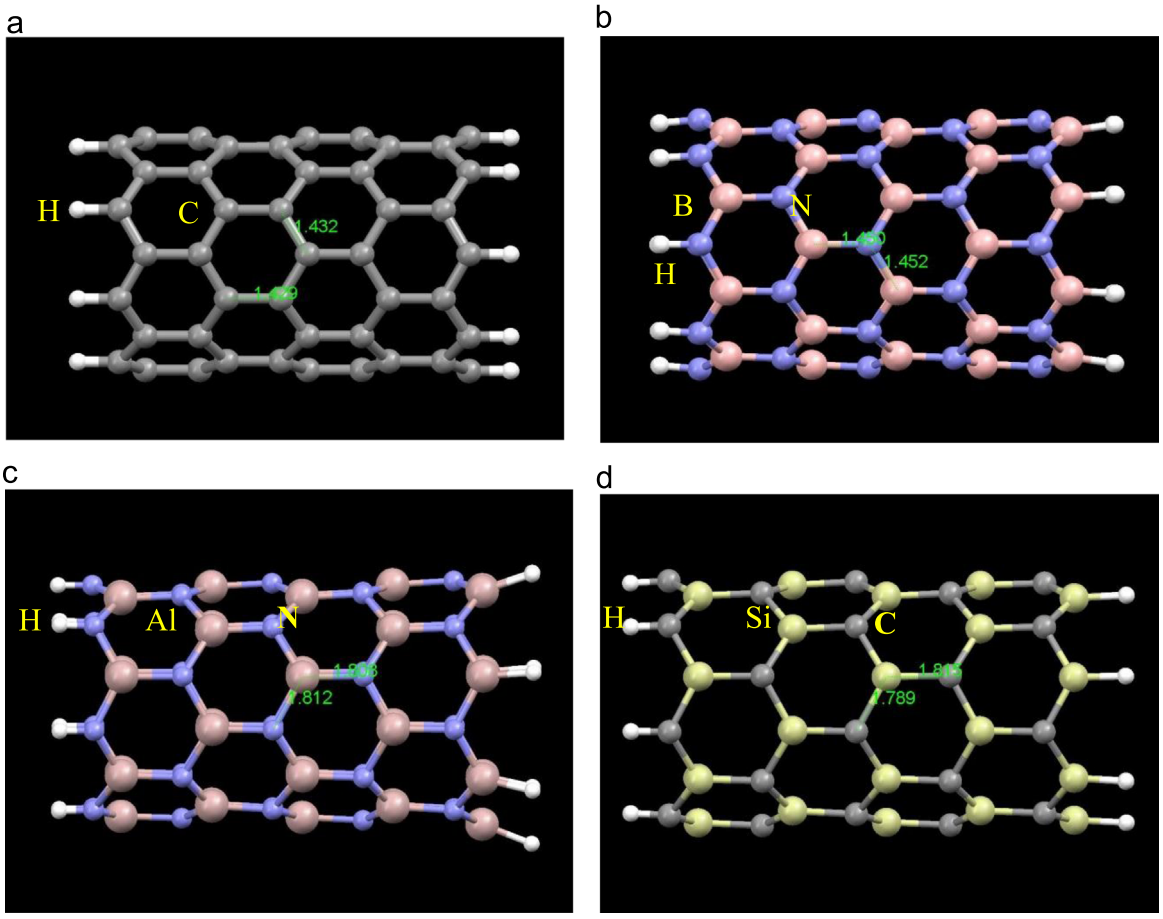

Fig. 1. Schematic representation of optimized geometric structures of (a) CNT, (b) BNNT, (c) AlNNT and (d) SiCNT and calculated bond lengths in Å.