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Boron-carbon Nanotube Modification Using Alkaline Metal Atoms

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In this paper we present the results of theoretical research into the properties of two types of boron-carbon nanotubes (BCNTs) within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme. We studied the mechanism of Li, K and Na atoms sorption on the external surface of single-walled BC_3 zig-zag nanotubes. We defined the optimal geometry of the sorption complexes and obtained the sorption energy values.

Keywords: Boron-carbon nanotubes, Ionic-built covalent-cyclic cluster model, Quantum chemical calculations, Adsorption, Metal superlattice.

PACS numbers: 61.46, 71.15

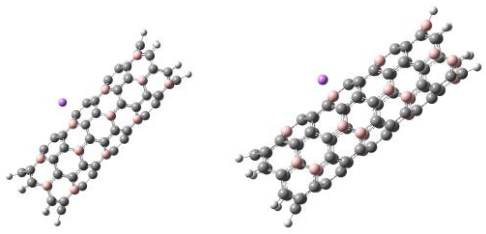
1. INTRODUCTION

The discovery of carbon NTs in the early nineties was followed by intensive investigation into their electronic structure and energy spectrum parameters as well as physical and chemical properties. Along with studying of nanotube properties researchers started searching for ways to modify NTs and fabricate structures having new mechanical, electronic and other properties. Due to high surface activity nanotubes can be used as basis for fabricating various types of composites. In particular, it was found that introduction of metal atoms between the tubulene layers leads to the formation of nanotube based composite structures such as hollow alternating metallic supercells, nanotube conductors in semiconducting coating, etc., that possess new conducting, magnetic and electrical properties [1].

2. THE NANOTUBE MODEL

2.1 Boron Carbon Nanotube Clusters

As geometrical models of the studied tubulenes we selected clusters containing six hexagon boron-carbon cycles located on the tube perimeter and four elementary layers located along the tube axis. Since a nanotube is an infinite structure hydrogen pseudo atoms were used to complete loose chemical bonds on the nanotube edge. A model of a covalent cyclic cluster built in via



a) b)

Fig. 1 – BC_3 nanotube (6,0) with an absorbed lithium atom on the nanotube surface: a) type A of C and B atoms positions; b) type B of C and B atoms positions

via ionic bonding in the framework of the semi-empirical quantum chemical MNDO calculation procedure was applied [1]. Two possible positions of carbon and boron atoms in respect to a lithium atom on the tube external surface in BC_3-tubulenes clusters are shown in Figure 1.

The present paper presents calculations of alkaline metal atoms (AM) (Li, Na, K) adsorption on the boron-carbon BC_3 nanotubes (6, 0) [2-10] type external surface with the view of exploring a possibility to fabricate boron-carbon nanotube based metal-phase composites.

2.2 Calculation Model

In order to eliminate the influence of boundary effects, we modelled the process so that adsorbed atoms (Li, K, Na) bound either to a carbon or boron atom located approximately in the middle of the boron-carbon nanotube cluster. The adsorption process for alkaline metal atoms was modeled in increments of 0,1 Å in the direction of the perpendicular to the tube axis passing through the boron or carbon atom on which the adsorption takes place. The geometrical parameters of the system were optimized in quantum-chemical calculations. Adsorption energy values were calculated as the difference between the total energy value of non-interacting adsorbent model of a corresponding atom and a related adsorption complex, Formula (1).

$$E_{ad} = E_{ad.k.} - (E_{tub} + E_{Me}) \quad (1)$$

3. RESULTS AND DISCUSSION

As a result of calculations we obtained the potential energy curves of these processes. Analysis shows that all the curves for the nanotubes reveal the presence of energy minimum that enabled us to conclude that atoms adsorbed on the BC_3 tubulene external surface formed stable adsorption complexes (Fig. 2-5). Adsorption energy values E_{ad} for Li, K, Na atoms and corresponding adsorption distances R_{ad} are shown in Table 1.

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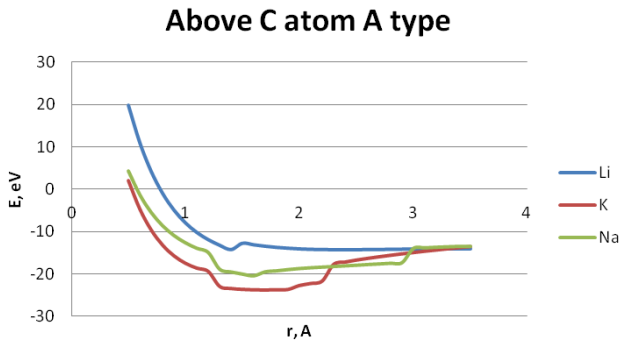

Fig. 2 – The energy curve of the alkaline metal atoms adsorption process on the boron-carbon nanotube A type (6, 0) external surface (a C atom)

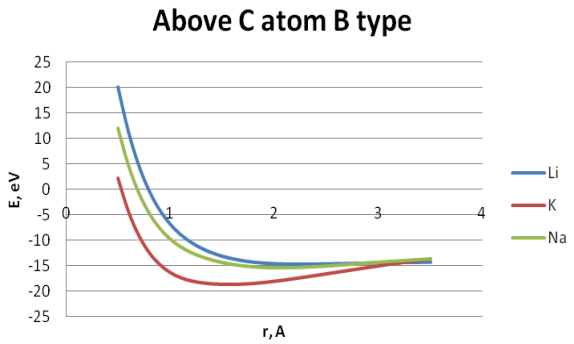

Fig. 4 – The potential energy curve of the alkaline metal atoms adsorption process on the boron-carbon nanotube B type (6, 0) external surface (a C atom)

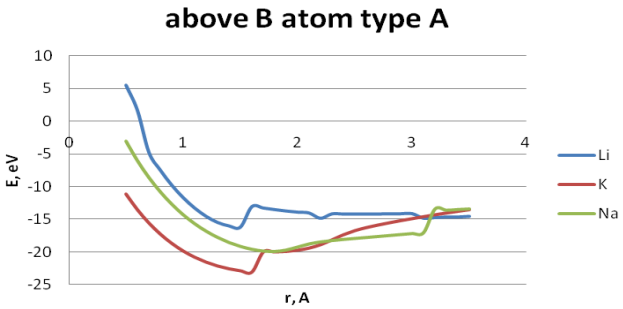

Fig. 3 – The potential energy curve of the alkaline metal atoms adsorption process on the boron-carbon nanotube A type (6, 0) external surface (a B atom)

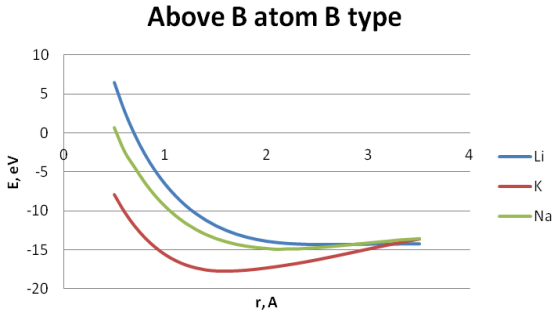

Fig. 5. – The potential energy curve of the alkaline metal atoms adsorption [process on the boron-carbon nanotube B type (6, 0) external surface (a B atom)

Table 1 – The adsorption energies E_{ad} for Li, K, Na atoms and corresponding adsorption distances R_{ad}. Letters C and B denote an approximation to boron and carbon atoms, respectively

	Li		K		Na	
	C	B	C	B	C	B
Type A						
E_{ad}, eV	14,21	15,97	23,73	23,13	20,33	19,94
R_{ad}, Å	1,4	1,4	1,7	1,6	1,6	1,8
Type B						
E_{ad}, eV	14,63	14,28	18,7	17,77	15,4	14,98
R_{ad}, Å	2,3	2,6	1,6	1,6	2,1	2,1

The charge distribution over the metal atoms indicates that electron transfer to boron and carbon atoms located on the nanotube external surface takes place, which increases the number of majority charge carriers in tubulenes; as a result BC3 nanotubes, which we had previously classified as narrow-gap semiconductor, begin to take on metallic properties (the occurrence of surface conductivity is attributed to electrons from metal atoms).

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