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On topological indices of tri-hexagonal boron nanotubes

I. NADEEM, H. SHAKER*
Department of Mathematics COMSATS Institute of Information Technology, Lahore Pakistan

Several chemical indices have been introduced in theoretical chemistry to measure the properties of molecular structures, such as atom bond connectivity (*ABC*) index and geometric-arithmetic (*GA*) index. Boron nanotubes are attractive because of their novel electronic properties due to the presence of multicenter bonds. Their thermal stability and mechanical properties are important issues in nanodevice applications and thus require intensive study. Y. Liu et al. [30] predicted a new class of boron nanotubes, called the Tri-Hexagonal boron nanotubes, which are constructed from triangles and hexagons. In this paper, we present the *ABC* index, the fourth version of *ABC* index, *GA* index and the fifth version of *GA* index for the Tri-Hexagonal boron nanotubes.

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1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools without necessarily referring to quantum mechanics [1-3]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [4]. This theory has an important effect on the development of the chemical sciences.

Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination. Such indices are widely used for establishing relationships between the structure of molecular graph and their physicochemical properties. Topological indices play a vital role in the study of the quantitative structure-activity relationship (QSAR) and the quantitative structure-property relationship (QSPR).

In mathematical chemistry, a molecular graph G is a simple graph such that its vertices correspond to the atoms and the edges to the bond. The degree of a vertex $v \in V(G)$ is the number of edges incident to v and denoted by $d_G(v)$. The distance between two vertices u and v is denoted as $d(u,v)$ and is the length of shortest path between u and v in graph G.

There are two major classes of topological indices, one is distance based and the other is degree based topological index. The notion of topological index was firstly introduced by Wiener [5] in 1947, while he was working on boiling point of paraffin. He named his index as *path number*. Later on, the path number was renamed as Weiner index and then theory of topological index started. The Wiener index is a distance based topological index and is defined as the sum of distances between all pairs of vertices in G.

The first degree based topological index is Randić connectivity index $\chi(G)$ introduced in 1975 by Milan Randić [6], who has shown this index to reflect molecular branching. Randić index is defined as

$$\chi(G) = \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

In 2009, Estrada et al. [7] introduced atom-bond connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes [7,8]. In [9], it was shown that ABC index can be used for modeling thermodynamic properties of organic chemical compounds. This index is defined as follows

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}}$$

Recently, Ghorbani et al. [10] introduced the fourth version of the atom-bond connectivity index (ABC_4) as follows

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{\delta_G(u) + \delta_G(v) - 2}{\delta_G(u)\delta_G(v)}}$$

where $\delta_G(u) = \sum_{uv \in E(G)} d_G(v)$ and $\delta_G(v) = \sum_{uv \in E(G)} d_G(u)$. The first Geometric Arithmetic connectivity index (or simply Geometric Arithmetic Index (GA) of a connected graph G was introduced by Vukičević et al. [11] in 2009 and is defined as

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

The reason for introducing a new index is to gain better prediction of properties of molecules. The predicting ability of the *GA* index compared with Randić index is reasonably better [11-12], for the prediction of physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and a centric factor. Hence, one can think that *GA* index should be considered in the QSAR/QSPR researches.

Recently fifth version of *GA* index (GA_5) is proposed by Graovac et al. [13] in 2011 and defined as

$$GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$

Nowadays *ABC* and *GA* indices are extensively studied by the researchers. The *ABC*, ABC_4, *GA* and GA_5 indices for carbon fullerene networks and carbon nanotube networks are discussed in [14]. For further study of these topological indices for various graph families, see [15-19].

In this paper, we study these topological indices for a newly introduced class of nanotubes fabricated from carbon nanotubes. This class of nanotubes called the Tri-Hexagonal boron nanotubes.

2. Tri-Hexagonal Boron Nanotube

The first boron triangular nanotubes were created in 2004 and formed from a triangular sheet [20-22]. The recent discovery of boron triangular nanotubes challenges the monopoly of carbon nanotubes (CNTs). Scientists believe that boron triangular nanotubes are better than carbon nanotubes [20,23,24]. Sohrab Ismail-Beigi [25] speculates that if a superconducting nano computer will ever built, it might have boron wiring. Lately scientists have justified this speculation by discovering the world's smallest superconductor using nano scale molecular superconducting boron wires [26]. Boron nanotubes also have some better properties compared to CNTs such as high chemical stability, high resistance to oxidation at high temperatures and are a stable wide band-gap semiconductor. Because of these properties, they can be used for applications at high temperatures or in corrosive environments such as batteries, fuel cells, super capacitors, high speed machines as solid lubricant [27]. The stability, mechanical and electronic properties of boron nanotubes has been discussed in [22, 28].

The boron triangular nanotubes are formed from CNTs by adding an extra atom to the center of each hexagon [29]. Y. Liu et al. [30] predicted a new class of boron nanotubes which are constructed from triangles and hexagons, called the Tri-Hexagonal boron nanotubes. These nanotubes are formed by removing some atoms from boron triangular nanotubes. These nanotubes are sparser than the other boron nanotubes and after relaxation it remains flat and metallic independent of their chirality. A three-dimensional perception of Tri-Hexagonal boron nanotube is shown in Fig. 1.

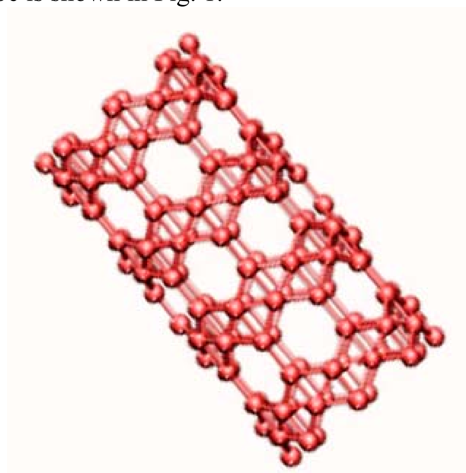

Fig. 1. Three-dimensional perception of Tri-Hexagonal boron nanotube.

We denote this nanotube by $C_3C_6(H)[p,q]$ where p is the number of hexagons in one column and q is the number of hexagons in one row in two-dimensional lattice of $C_3C_6(H)[p,q]$ nanotube. This nanotube has $8pq$ number of vertices and $q(18p-1)$ number of edges. The graph of $C_3C_6(H)[p,q]$ nanotube is shown in the Fig. 2.

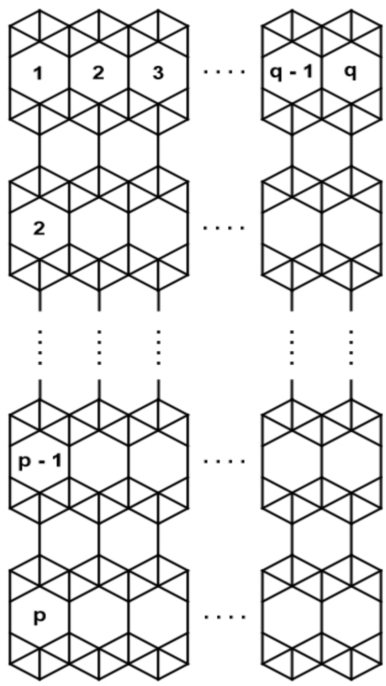

Fig. 2. The graph of $C_3C_6(H)[p,q]$ nanotube.

3. Main Results

In this section, we present our main results. In the following, we determine *ABC* index and fourth version of *ABC* index of $C_3C_6(H)[p,q]$ nanotube.

Theorem 1. *Consider the Tri-Hexagonal boron nanotube* $C_3C_6(H)[p,q]$ *, then*

$$ABC\left(C_3C_6(H)[p,q]\right)=\left(\frac{5\sqrt{30}+60\sqrt{7}+16\sqrt{10}}{10\sqrt{5}}\right)pq+\left(\frac{24\sqrt{2}-\sqrt{30}-12\sqrt{7}}{4\sqrt{5}}\right)q$$

Proof. Consider the Tri-Hexagonal boron nanotube $G=C_3C_6(H)[p,q]$. There are four partitions of edge set correspond to their degree of end vertices which are

$$E_1=\{uv\in E(G)\mid d_G(u)=3 \text{ and } d_G(v)=5\}$$
$$E_2=\{uv\in E(G)\mid d_G(u)=d_G(v)=4\}$$
$$E_3=\{uv\in E(G)\mid d_G(u)=4 \text{ and } d_G(v)=5\}$$
$$E_4=\{uv\in E(G)\mid d_G(u)=d_G(v)=5\}$$

The representatives of these partite sets are shown in Figure 3, in which red, green, black and blue edges are edges belong to E_1, E_2, E_3 and E_4 respectively.

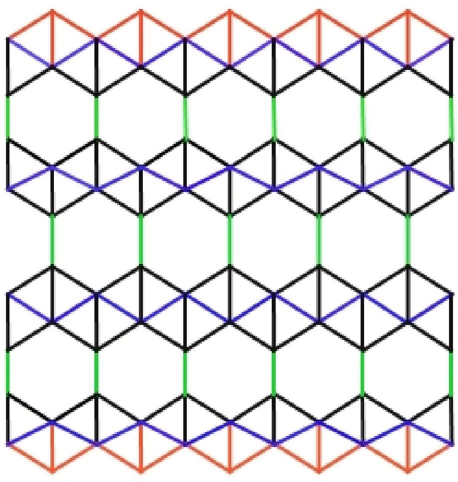

Fig. 3. The graph of $C_3C_6(H)[p,q]$ nanotube with p=2 and q=5.

The Table 1 shows the partition of edge set of G correspond to their degree of end vertices.

Table 1: The edge partition of G correspond to degree of end vertices.

$(d_G(u),d_G(v))$	Number of Edges
(3,5)	*6q*
(4,4)	*q(2p-1)*
(4,5)	*6q(2p-1)*
(5,5)	*4pq*

Now we apply the formula of ABC to compute this index for G.

$$\begin{aligned}ABC(G)&=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}\\&=\sum_{uv\in E_1}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}+\sum_{uv\in E_2}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}\\&+\sum_{uv\in E_3}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}+\sum_{uv\in E_4}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}\\&=(6q)\sqrt{\frac{3+5-2}{3\times5}}+q(2p-1)\sqrt{\frac{4+4-2}{4\times4}}\\&+6q(2p-1)\sqrt{\frac{4+5-2}{4\times5}}+4pq\sqrt{\frac{5+5-2}{5\times5}}\end{aligned}$$

After simplification, we get

$$ABC(G)=\left(\frac{5\sqrt{30}+60\sqrt{7}+16\sqrt{10}}{10\sqrt{5}}\right)pq+\left(\frac{24\sqrt{2}-\sqrt{30}-12\sqrt{7}}{4\sqrt{5}}\right)q$$

The fourth version of ABC index for $C_3C_6(H)[p,q]$ nanotube is computed as follows.

Theorem 2. *Consider the Tri-Hexagonal boron nanotube* $C_3C_6(H)[p,q]$ *, then*

$$\begin{aligned}ABC_4\left(C_3C_6(H)[p,q]\right)&=\left(\frac{12\sqrt{39}}{\sqrt{418}}+\frac{2\sqrt{42}}{11}+\frac{12}{19}\right)pq\\&+\left(\frac{2\sqrt{34}}{3\sqrt{35}}+\frac{2\sqrt{37}}{\sqrt{95}}+\frac{4\sqrt{38}}{\sqrt{399}}+\frac{2\sqrt{13}}{\sqrt{35}}\right)q\\&+\left(\frac{2\sqrt{11}}{5}-\frac{12\sqrt{39}}{\sqrt{418}}-\frac{2\sqrt{42}}{11}-\frac{6}{19}\right)q\end{aligned}$$

Proof. Consider the Tri-Hexagonal boron nanotube $G=C_3C_6(H)[p,q]$. There are eight partitions of the edge set correspond to their degree sum of neighbors of end vertices which are

$E_1 = \{uv \in E(G) \mid \delta_G(u) = 15 \text{ and } \delta_G(v) = 20\}$
$E_2 = \{uv \in E(G) \mid \delta_G(u) = 15 \text{ and } \delta_G(v) = 21\}$
$E_3 = \{uv \in E(G) \mid \delta_G(u) = \delta_G(v) = 19\}$
$E_4 = \{uv \in E(G) \mid \delta_G(u) = 19 \text{ and } \delta_G(v) = 20\}$
$E_5 = \{uv \in E(G) \mid \delta_G(u) = 19 \text{ and } \delta_G(v) = 21\}$
$E_6 = \{uv \in E(G) \mid \delta_G(u) = 19 \text{ and } \delta_G(v) = 22\}$
$E_7 = \{uv \in E(G) \mid \delta_G(u) = 20 \text{ and } \delta_G(v) = 21\}$
$E_8 = \{uv \in E(G) \mid \delta_G(u) = \delta_G(v) = 22\}$

The representatives of these partite sets are shown in Figure 4, in which red, sky blue, green, purple, pink, black, yellow and blue edges are the edges belong to E_1, E_2, E_3, E_4, E_5, E_6, E_7 and E_8 respectively.

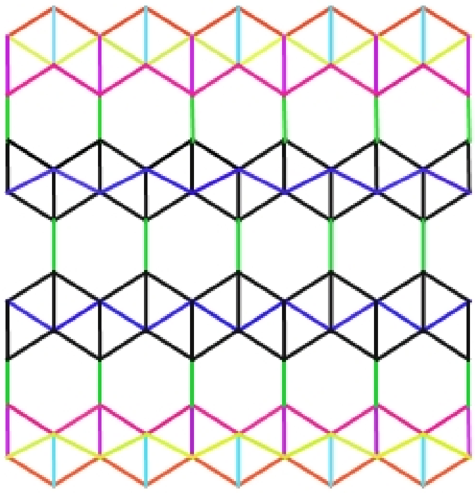

Fig. 4. The graph of $C_3C_6(H)[p,q]$ nanotube with p=2 and q=5.

The Table 2 shows the partition of edge set of G correspond to their degree sum of neighbors of end vertices.

Table 2: The edge partition of G correspond to degree sum of neighbors of end vertices.

$(\delta_G(u), \delta_G(v))$	Number of Edges
(15,20)	$4q$
(15,21)	$2q$
(19,19)	$q(2p-1)$
(19,20)	$2q$
(19,21)	$4q$
(19,22)	$12q(p-1)$
(20,21)	$4q$
(22,22)	$4q(p-1)$

Now we apply the formula of ABC_4 to compute this index for G.

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$= \sum_{uv\in E_1} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{uv\in E_2} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$+ \sum_{uv\in E_3} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{uv\in E_4} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$+ \sum_{uv\in E_5} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{uv\in E_6} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$+ \sum_{uv\in E_7} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{uv\in E_8} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$= 4q\sqrt{\frac{15+20-2}{15\times 20}} + 2q\sqrt{\frac{15+21-2}{15\times 21}}$$

$$+q(2p-1)\sqrt{\frac{19+19-2}{19\times 19}} + 2q\sqrt{\frac{19+20-2}{19\times 20}}$$

$$+4q\sqrt{\frac{19+21-2}{19\times 21}} + 12q(p-1)\sqrt{\frac{19+22-2}{19\times 22}}$$

$$+4q\sqrt{\frac{20+21-2}{20\times 21}} + 4q(p-1)\sqrt{\frac{22+22-2}{22\times 22}}$$

After simplification, we get

$$ABC_4(G) = \left(\frac{12\sqrt{39}}{\sqrt{418}} + \frac{2\sqrt{42}}{11} + \frac{12}{19}\right)pq$$
$$+\left(\frac{2\sqrt{34}}{3\sqrt{35}} + \frac{2\sqrt{37}}{\sqrt{95}} + \frac{4\sqrt{38}}{\sqrt{399}} + \frac{2\sqrt{13}}{\sqrt{35}}\right)q$$
$$+\left(\frac{2\sqrt{11}}{5} - \frac{12\sqrt{39}}{\sqrt{418}} - \frac{2\sqrt{42}}{11} - \frac{6}{19}\right)q$$

In the next theorem, we compute geometric-arithmetic (GA) index of $C_3C_6(H)[p,q]$ nanotube.

Theorem 3. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, then*

$$GA\left(C_3C_6(H)[p,q]\right) = \left(\frac{16\sqrt{5}+18}{3}\right)pq$$
$$+\left(\frac{9\sqrt{15}-16\sqrt{5}-6}{6}\right)q$$

Proof. Consider the Tri-Hexagonal boron nanotube $G = C_3C_6(H)[p,q]$. From Table 1, we have the partition of edge set of G correspond to their degree of end vertices. Now we apply the formula of GA to compute this index for G.

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$
$$=\sum_{uv\in E_1}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}+\sum_{uv\in E_2}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$
$$+\sum_{uv\in E_3}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}+\sum_{uv\in E_4}\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$
$$=(6q)\frac{2\sqrt{3\times 5}}{3+5}+q(2p-1)\frac{2\sqrt{4\times 4}}{4+4}$$
$$+6q(2p-1)\frac{2\sqrt{4\times 5}}{4+5}+(4pq)\frac{2\sqrt{5\times 5}}{5+5}$$

After simplification, we get

$$GA(G)=\left(\frac{16\sqrt{5}+18}{3}\right)pq+\left(\frac{9\sqrt{15}-16\sqrt{5}-6}{6}\right)q$$

The fifth version of *GA* index is computed in the following theorem.

Theorem 4. *Consider the Tri-Hexagonal boron nanotube* $C_3C_6(H)[p,q]$ *, then*

$$GA_5\left(C_3C_6(H)[p,q]\right)=$$
$$\left(\frac{24\sqrt{418}}{41}+6\right)pq+\left(\frac{16\sqrt{3}}{7}+\frac{\sqrt{35}}{3}\right)q$$
$$+\left(\frac{8\sqrt{95}}{39}+\frac{8\sqrt{399}}{40}+\frac{16\sqrt{105}}{41}+\frac{24\sqrt{418}}{41}-5\right)q$$

Proof. Consider the Tri-Hexagonal boron nanotube $G=C_3C_6(H)[p,q]$. From Table 2, we have the partition of edge set of *G* correspond to their degree sum of neighbors of end vertices.

Now we apply the formula of GA_5 to compute this index for *G*.

$$GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$
$$=\sum_{uv\in E_1}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}+\sum_{uv\in E_2}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$
$$+\sum_{uv\in E_3}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}+\sum_{uv\in E_4}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$
$$+\sum_{uv\in E_5}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}+\sum_{uv\in E_6}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$
$$+\sum_{uv\in E_7}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}+\sum_{uv\in E_8}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$
$$=4q\frac{2\sqrt{15\times 20}}{15+20}+2q\frac{2\sqrt{15\times 21}}{15+21}$$
$$+q(2p-1)\frac{2\sqrt{19\times 19}}{19+19}+2q\frac{2\sqrt{19\times 20}}{19+20}$$
$$+4q\frac{2\sqrt{19\times 21}}{19+21}+12q(p-1)\frac{2\sqrt{19\times 22}}{19+22}$$
$$+4q\frac{2\sqrt{20\times 21}}{20+21}+4q(p-1)\frac{2\sqrt{22\times 22}}{22+22}$$

After simplification, we get

$$GA_5(G)=\left(\frac{24\sqrt{418}}{41}+6\right)pq+\left(\frac{16\sqrt{3}}{7}+\frac{\sqrt{35}}{3}\right)q$$
$$+\left(\frac{8\sqrt{95}}{39}+\frac{8\sqrt{399}}{40}+\frac{16\sqrt{105}}{41}+\frac{24\sqrt{418}}{41}-5\right)q$$

4. Conclusions

Topological indices play a vital role in the study of physicochemical properties of chemical compounds. Degree based topological indices have got a prominent place in this study due to prediction of various chemical properties such as stability, enthalpy etc. with high predictive power. To compute and study these topological indices for various nanostructures is a respected problem in nanotechnology. In this study, we compute various degree based topological indices of Tri-Hexagonal boron nanotubes. These results give valuable information regarding chemical properties of these nanotubes.

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*Corresponding author: hani.uet@gmail.com