ISSN: 2230-9926

Available online at http://www.journalijdr.com

IJDR

International Journal of Development Research
Vol. 5, Issue, 05, pp. 4428-4431, May, 2015

International Journal of
DEVELOPMENT RESEARCH

Full Length Research Article

INTERACTION OF WATER ON BORON NITRIDE FULLERN LIKE-STRUCTURS: A COMPUTATIONAL STUDY

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ARTICLE INFO

Article History:

Received 25th February, 2015
Received in revised form
29th March, 2015
Accepted 10th April, 2015
Published online 31st May, 2015

Key words:

Boron nitride nano cluster,
Density functional theory,
Adsorption,
H_2O.

ABSTRACT

Interaction of H_2O molecule and BN fullerene like structures was studied based on the density functional theory. The H_2O molecule is adsorbed on the surface of BN fullerene like structures. All calculations were performed using DFT within M062X method and has been widely used in the nanostructure studies. 6-311G** all electron basis sets were used for the optimization, frontier molecular orbital (FMO) analyses, and energy calculations. The adsorption energies of H2O on $B_{16}N_{16}$ and $B_{24}N_{24}$ fullerene – like structures via O to B atoms were estimated to ranging from -0.694 eV to -0.923 eV and -0.459 eV to -0.605 eV respectively, and via H atoms of H2O to B atoms were estimated to ranging from -0.694 eV to -0.921 eV and -0.593eV to -0.599 eV respectively. The most stable adsorption configurations are those in which the O or H atoms of H_2O are adsorbed to the B atoms of $B_{16}N_{16}$ and $B_{24}N_{24}$ fullerenes – like structures. The HOMO-LUMO gap of H_2O adsorption energies on BN fullerene like structures i.e. $B_{16}N_{16}$ and $B_{24}N_{24}$ are about 8.90 eV and 8.58 eV has reduced by as much as 0.21eV and 0.17 eV compared to that of the pristine $B_{16}N_{16}$ and $B_{24}N_{24}$ respectively.

INTRODUCTION

The water is the source of life and is the most abundant compound on Earth's surface and more than 75 percent of the body's mass of a man is composed of water and more than 70 percent of the Earth's surface is covered by water. Furthermore, if the usage of boron nitride fullerenes like be considered in critical systems, you will find applications such as pharmaceutical carriers, insulation, sensors and etc. for them. The interaction of the substance with water will be great importance. The study of water adsorption on the various materials have been investigated (Hugo E Romero *et al*., 2009; Beheshtian *et al*., 2012. Recently, the molecular encapsulation of water inside the nanoscale channels such as the CNTs and BNNTs have been intensively studied (Murata *et al*., 2000; Koga *et al*., 2001; Hummer *et al*., 2001; Kolesnikov *et al*., 2004; Gogotsi *et al*., 2001; Holt *et al*., 2006; Naguib *et al*., 2004; Majumder *et al*., 2005; Zhao *et al*., 2008; Mashl *et al*., 2003; Feng *et al*., 2007; Rasaiah *et al*., 2008; Byl *et al*., 2006; Maniwa *et al*., 2007; Takaiwa *et al*., 2008 and Hanasaki *et al*., 2008). Since determination of water behavior in nanoscale environment is important for biological activities of macromolecules, study of the water interaction with substrate molecules is of great interest. Therefore, numerous experimental (Byl *et al*., 2006 and Ellison *et al*., 2005) and theoretical (Zangi, 2004 and Gelb *et al*., 1999) works have been devoted to study the encapsulation of water chains inside the nanoscale channels.

However, due to the extended hydrogen bonding network, it is not easy to obtain a molecular scale description of liquid and solid water. Hence, exploring the structural and binding properties of small water clusters are almost the first step of understanding the properties of bulk water. To this aim, several theoretical studies have been carried out to investigate the strength of the hydrogen bonds and their cooperatives (Muller-Dethlefs and Hobza, 2000 and Ugalde *et al*., 2000). Recently, (Won and Aluru, 2007, 2008) showed that the BNNTs exhibit superior water-filling behaviors because of the comparatively hydrogen bonding interactions between the nitrogen atoms of the BNNT and the water molecules. Zeng and co-workers (An *et al*., 2007) also studied the adsorption of a single water molecule on the pristine and stone-wales defect BNNTs through density functional theory (DFT) calculations. The effect of water molecule adsorption on the surface of (5,0)

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zigzag boron nitride nanotube was studied by density functional theory calculations(Beheshtian Javad *et al*., 2010).

A detailed understanding of surface structure is of great importance in surface science, heterogeneous catalysis, nanoscience, and such other technologies. Bonding of simple atoms and molecules such as NH_3, CO, NO, and alkali metals to metal oxides is one of the serious challenges in theoretical studies (Hoeft *et al*., 2001; Kittel *et al*., 2002 and Rappold and Luft, 1999). The structural and electronic properties of chemical modification of pristine and Na-doped MgONTs with NH_3 and H2O molecules have been investigated, on the basis of density functional theory calculations (Beheshtianand *et al*., 2013). Therefore, here we study the interaction of water with two structures i.e. $B_{16}N_{16}$ and $B_{24}N_{24}$.

RESULTS AND DISCUSSION

The water molecule, $B_{16}N_{16}$ and $B_{24}N_{24}$ were optimized via M062X method and basis set 6-311G ** then the water molecule near the surface structures of $B_{16}N_{16}$ and $B_{24}N_{24}$ also were optimized via previously mentioned method and basis set in the above. Water molecule can be placed on the different states on the surface of these structures, we study these scenarios. These are: a) Approaching of the water from the hydrogen on the nitrogen atom structures, b) water is approaching from the hydrogen's head on the nitrogen atom structures, c) approaching the water from the hydrogen on the boron atom structures and d) Approaching of the water from theside of oxygen atom on the boron atom in $B_{16}N_{16}$ and $B_{24}N_{24}$ structures. In this calculation,while optimizing of energy all the parameters of geometric structures, have beenchangeable and no limits are set.

Since in the seventeen case that we studied, the oxygen atom of the water molecule with boron atom or from their hydrogen atoms with boron of the $B_{16}N_{16}$ have interacted. The results interaction in sixteen states of water molecules with the oxygen atom of boron were similar, so only results from these two modes and one mode of interaction of water molecules from the hydrogen atom head, with boron atom of the $B_{16}N_{16}$ have been reported.

Table 1.Geometric data for different structures, bond length according to Å

Configuration	Structures	Diameter (Å)	B-N(Å)
-	$B_{16}N_{16}$	5.89	1.43
-	$B_{24}N_{24}$	6.67	1.42
A_1	$B_{16}N_{16}$-H_2O-1B-33O	5.90	1.49
A_2	$B_{16}N_{16}$-H_2O -18B-33O	5.90	1.49
B_1	$B_{16}N_{16}$-H_2O -1B-34H	5.91	1.49
C_1	$B_{24}N_{24}$-H_2O-1B-49O	6.63	1.48
D_1	$B_{24}N_{24}$-H_2O-1B -50H	6.62	1.47

In twenty-six cases that we studied on water adsorption on the $B_{24}N_{24}$, since the optimal structures have the similar energy that these related to twenty-one modes that water molecules through their oxygen atoms with boron atom of $B_{24}N_{24}$ structure and five state which attract water molecules resume their hydrogen atoms are with boron atom in $B_{24}N_{24}$ structure, two results have been reported.All the structures after optimization and the HOMO and LUMO molecular orbitals structures are shown in Figure 1. The DOS curves plotted are displayed in Figure 2. The results of the calculations are listed in two tables, Table 1 and Table 2. Table 1 shows the data geometric structures.

Table 2.Adsorption energy Data (eV), HOMO-LUMO (au), the energy gap in terms of (eV), dipole moments in terms of (Debye) and the amount of charge transfers from H_2O to $B_{16}N_{16}$ and $B_{24}N_{24}$ molecule in terms of the electron (e) water (Q_{H2O} from left to right respectively

Structures or Configuration	E_{ads}(eV)	HOMO	LUMO	Gap(eV)	dipole	Q_{H2O} (electron)
$B_{16}N_{16}$	-	-0.348	-0.014	9.11	0.008	-
$B_{16}N_{16}$-$H_2O(A_1)$	-0.923	-0.326	-0.003	8.95	6.166	0.257
$B_{16}N_{16}$-$H_2O(A_2)$	-0.695	-0.330	-0.002	9.03	5.689	0.272
$B_{16}N_{16}$-$H_2O(B_1)$	-0.921	-0.326	-0.003	8.89	6.156	0.290
$B_{24}N_{24}$	-	-0.337	-0.015	8.76	0.005	-
$B_{24}N_{24}$-H_2O-1B-49O(C_1)	-0.596	-0.322	-0.006	8.60	5.901	0.257
$B_{24}N_{24}$-H_2O-1B-50H(D_1)	-0.593	-0.006	-0.322	8.61	5.888	0.257

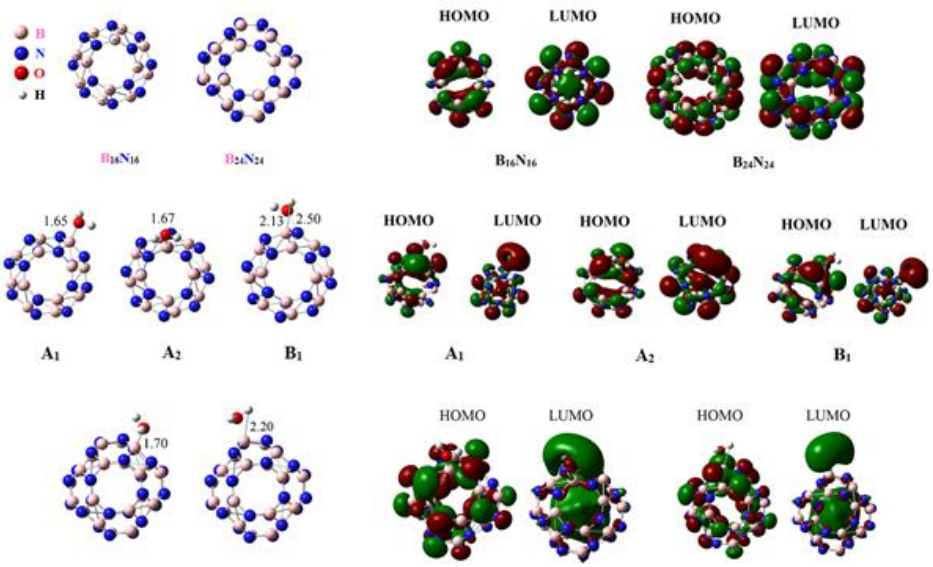

Figure 1.Optimized structure of stable $B_{16}N_{16}$ and B_{24} N_{24} & water adsoption on $B_{16}N_{16}$ and $B_{24}N_{24}$ (in the left). HOMO and LUMO MOs for $B_{16}N_{16}$ and $B_{24}N_{24}$ and adsorption of H_2O Molecule on BN nanostructures (in theright)

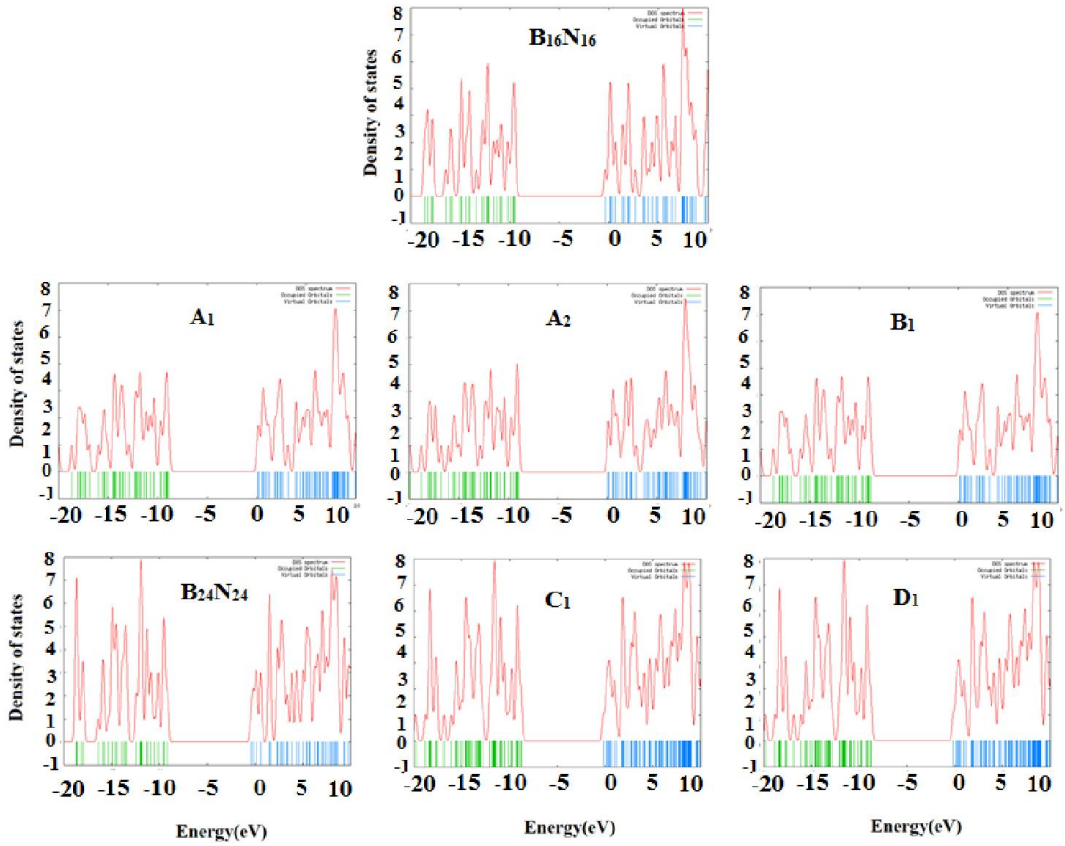

Figure 2.Density states for $B_{16}N_{16}$ and $B_{24}N_{24}$& water adsoption on $B_{16}N_{16}$ and $B_{24}N_{24}$

Table 2 demonstrates adsorption energy (eV), the energy levels of the HOMO and LUMO (au), the dipole moments (Debye), the amount of charge transferred (electron) respectively. The results of Table 1and Table 2 and Figure 1 and Figure 2 shows that the adsorption distance of H_2O molecules and the $B_{16}N_{16}$ structure is almost identical between A_1 and A_2, but in the B_1 mode it is more than A_1 and A_2. But the adsorption energy in the case of A_2 is less than A_1 and in the B_1 mode, the adsorption energy is more than A_2. Table 1 shows that after adsorption of water on the $B_{16}N_{16}$ structure the B-N bond is longer than pristine $B_{16}N_{16}$. Also it is seen slightly increasing in diameter of $B_{16}N_{16}$ after adsorption of water on it.Since the results of the adsorbed energy are in the range between 0.2 and 0.7 electron volt in gas phase so it is in the range of physically adsorbed approximately 0.6 eV on $B_{24}N_{24}$, whereas it is a little more than 0.6 i.e. approximately 0.9 on $B_{16}N_{16}$. It is deduced that water molecule adsorption on $B_{16}N_{16}$ is much power than a physical adsorption while water molecule adsorption on $B_{24}N_{24}$ is in the rangeof physical adsorption.

Conclusions

Since the results of the adsorbed energy are in the range between 0.2 and 0.7 electron volt in gas phase so it is in the range of physically adsorbed approximately 0.6 eV on $B_{24}N_{24}$, whereas it is a little more than 0.6 i.e. approximately 0.9 on $B_{16}N_{16}$. It is deduced that water molecule adsorption on $B_{16}N_{16}$ is much power than a physical adsorption while water molecule adsorption on $B_{24}N_{24}$ is in the rangeof physical adsorption.

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