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Investigation Adsorption Tyrosine on Surface Single Walled Aluminum –Nitride and Doped-Si Aluminum-Nitride

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ABSTRACT

In this study, adsorption behavior of a tyrosine molecule on the external surface of Aluminum nitride Nanotubes and aluminum nitride which have seen with one silica atom by using Density Functional theory (DFT) has been studied. We can mention the optimized energy, NMR, NBO, changes in bond length from calculated parameters in this study in the gas phase and solvent phase. Bond energy shows that adsorption of the molecule on the aluminum nitride nanotube hybrid by silica atom is better than pure aluminum nitride nanotube and it can be proved, according to the results of NMR, NBO. The software used in this calculation, software Gauss view are Gaussian. According to results of a seen aluminum nitride nanotube with a silica atom that can be used in transferring of molecule tyrosine. Obtained energy for transferring tyrosine molecule is by aluminum nitride nanotube (-9554.0617 hartree) and energy for transferring tyrosine molecule is by a seen aluminum nitride nanotube with a silica atom (-9554.123 hartree).

Keywords: Adsorption; Aluminum nitride Nanotubes; Tyrosine drug; Density functional theory

1. INTRODUCTION

The use of nanomaterials and nanostructures has been extensively developed due to their special physical and chemical properties. The effect of substituting one atom for another for nanotubes (aluminum or nitrogen, which is called viscosity or hybridization) is also examined. In this study, the effect of tyrosine molecule adsorption on the surface of aluminum nitride and aluminum nitride nanotubes observed with silica atoms instead of an aluminum atom was investigated. In fact, the is to investigate the rate of adsorption by an aluminum hybrid with a silica atom. [1]

For software simulation of molecules, many software are used, which according to the purpose of the simulation, for

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example, for drug transfer, Gromex software works better than Hex and Gauss View software, because Gromex performs calculations in the solvent phase, but the software other calculations are performed in the gas and vacuum phases. The software we have used in this project are the model Nano-tube software, Gauss View and Gaussian. [2]The effect of iron atom on the structural and electronic properties of aluminum nitride nanotubes has been investigated. [3]In this research, the ability of aluminum nitride nanostructures (Nanocone, nanotubes and nanowires) to store hydrogen by the density theory function has been investigated. [4]The researcher investigated the effect of Bernanos's electric fields on single-walled aluminum nitride tubes (6, 0). Based on the field structures of electronic energy, aluminum nitride nanotubes saturated with hydrogen atoms are obtained by the density theory function. In this work, by optimizing the structure of nanotubes with the base method and series B3lyp / 6-31G * bipolar moment parameters, changes in atomic loads and total energy of nanotubes with different field effects were obtained. These parameters show that with increasing external field effects at the nanotube level, its applications also increase. Energy gap decreases with increasing field effects. [5]

The adsorption of nitrogen monoxide on the surface of pure aluminum nitride nanotubes and nanotubes of aluminum nitride seen with silica atoms has been investigated. One of the parameters studied in this research is nitrogen monoxide adsorption energy on the surface of nanotubes and the study of electronic and geometric properties of nanotubes due to nitrogen monoxide adsorption. In this work, it was found that the adsorption of monoxide was better in terms of oxygen. [6]The electronic properties of zigzag aluminum-gallium nitride nanotubes were compared with the armature type and it was found that in gallium nitride aluminum nanotube the zigzag type conductor has a direct relationship with the energy gap. The relationship is indirect. [7]The adsorption of carbon monoxide on the surface of aluminum nitride nanotubes has been investigated by field effects. [8]The adsorption properties of dinitrogen oxide on the surface of boron-nitride nanotubes (6, 0), (7, 0), (8, 0) have been investigated using quantum calculations. [9]

COMPUTATIONAL METHODS

In this project, three molecules of aluminum nitride nanotube, aluminum nitride diluted with silica atom and tyrosine molecule are used, which we will examine in the following.

In this project, aluminum nitride nanotubes (6,0) with a length of 12 (4 loops) which includes 30 nitrogen atoms and 30 aluminum atoms as well as 12 hydrogen atoms at the two free ends of the nanotube are used using Vegos View modeler nanotube software. Has been made and optimized. After optimizing this nanotube, we replaced one of the aluminum atoms with a silica atom and optimized it again.

Tyrosine molecule is an organic molecule that has a benzene ring, the shape of which is plotted using Gaussian software and then optimized with Gaussian software and quantum computing. To be obtained.

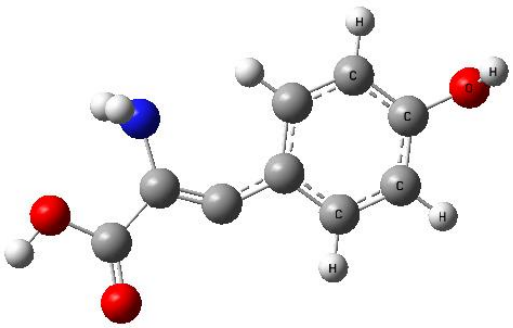
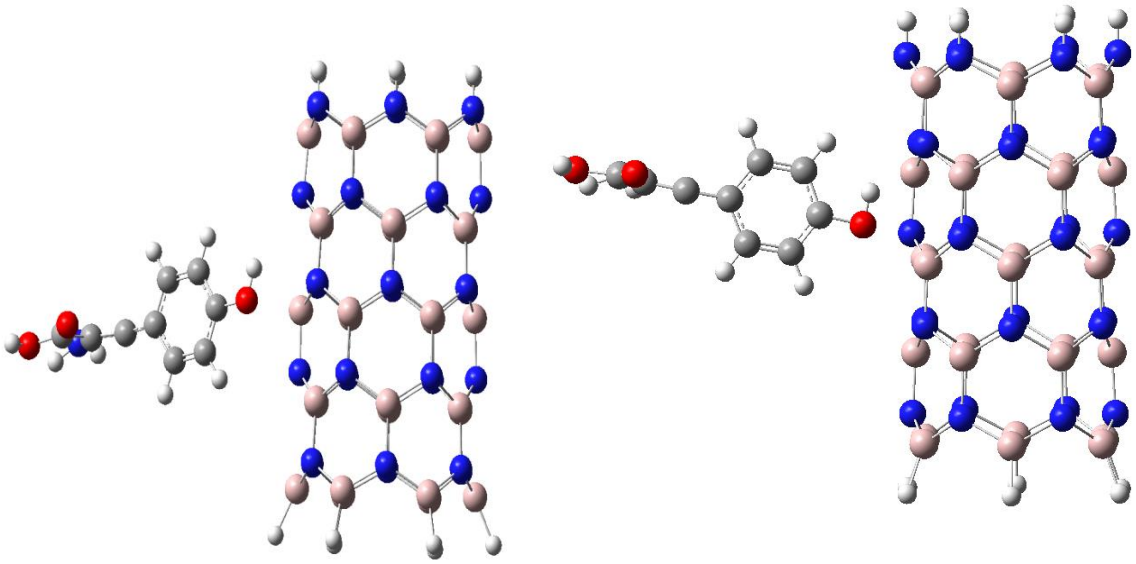


Fig. 1. Tyrosine molecule.

Experience has shown that accurate optimization calculations are necessary to find stable structures of a molecule. In this method, the wave and energy function for the initial structure is calculated. The optimization operation then proceeds to reach a new structure with less energy, and this process is repeated until we reach the structure with the least energy relative to the starting point. At each stage, complex algorithms are used to select a new structure and converge to the structure with the least energy.



(a) (b)

Fig. 2. Adsorption of tyrosine in terms of alcoholic oxygen on the surface of aluminum nitride nanotube in terms of a) aluminum b) nitrogen.

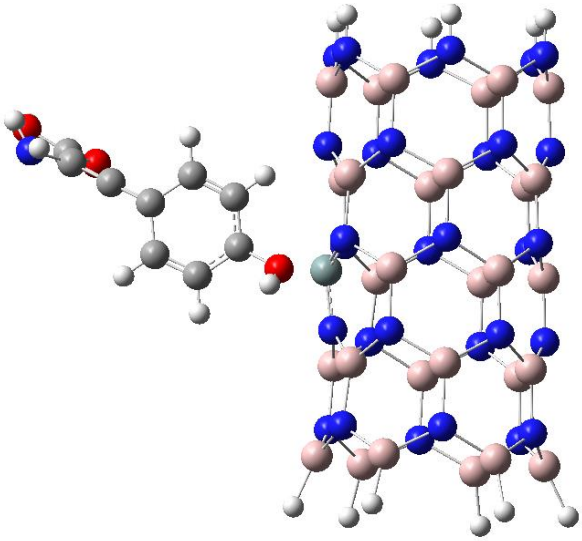


Fig. 3. Adsorption of tyrosine molecule in the direction of alcoholic oxygen on the surface of aluminum nitride nanotubes hybridized with silica atoms.

Reactions between solvent and solute play a special role in chemical and biochemical processes. Numerical self-consistent reaction field (SCRF) is used to obtain the adsorption energy in the solvent phase. This keyword requires that calculations in the presence of solvent be used. Tie the extruder model to be implemented in the polarized continuum model (overlapping spheres) by Thomas et al. Solvents are read as two real numbers in free form in a line of internal flow. The appropriate radius of solubility is calculated by calculating the molecular volume of the gas phase (in a separate step). If the solvent is not specified, the water solvent is considered by default. In the solvent phase, for this purpose, after optimizing the structure of the molecules, it is necessary to examine them in the solvent phase, which uses the following command to investigate the effects of the solvent on the molecules:

Method / basis set scf = tight scrf = (pcm, read, solvent = water) test

Nuclear magnetic resonance was first discovered in 1946 independently by Felix Bloch of Stanford University and Edward of Harvard University. Adsorption of electromagnetic radiation as a result of more transfer of nuclear energy in a strong magnetic field And this effect can be related to the structure of the molecule. Since then, the growth of the magnetic resonance spectroscopy method has been explosive, and this method has had a significant effect on the development of chemistry and biochemistry. Some nuclei, like electrons, rotate around their own axis. In the presence of an external magnetic field, a rotating nucleus has only a small number of stable orientations. Magnetic resonance of the nucleus occurs when a spinning nucleus absorbs enough electromagnetic radiation in the presence of a magnetic field of one orientation. With lower energy be excited to a higher energy orientation. Nuclear magnetic resonance spectroscopy involves measuring the amount of energy required to change spin nuclei from a stable orientation to a more unstable orientation in a magnetic field. Since spin nuclei in a magnetic field change direction at different frequencies, Different frequencies of adsorption radiation are required to change the orientation of the spin nuclei. The frequency at which the adsorption takes place is used for analysis and spectroscopy. Nuclear magnetic resonance has been shown to be a suitable tool for explaining the structural and electronic properties of most carbon materials. In addition to magnetic dipole torque, nuclei with spins larger than one also have electrical quadruple torque. The purpose of calculating this parameter is to investigate the isotropic and anisotropic loads of nanotubes due to the adsorption of tyrosine molecules.

To draw Nano-tubes, we can use the model Nano-tube software or via the Internet from the following website address:

www.html.tubegenonline/research/turin.nss.udel.edu

Create it with the appropriate bond and length and then add hydrogen atoms at both ends of the nanotube using Gauss View software. By applying optimization to a hypothetical structure, the original structure is changed and a new configuration is formed. We study the computational properties on the middle regions of nanotubes. Tyrosine, download its shape from the Internet, then draw it in Gauss View software, and after optimizing it in Gaussian software, using Gauss View software, open the optimized molecules and copy the tyrosine molecule next to the aluminum nitride nanotube. And examines the effects of their adsorption Let us.

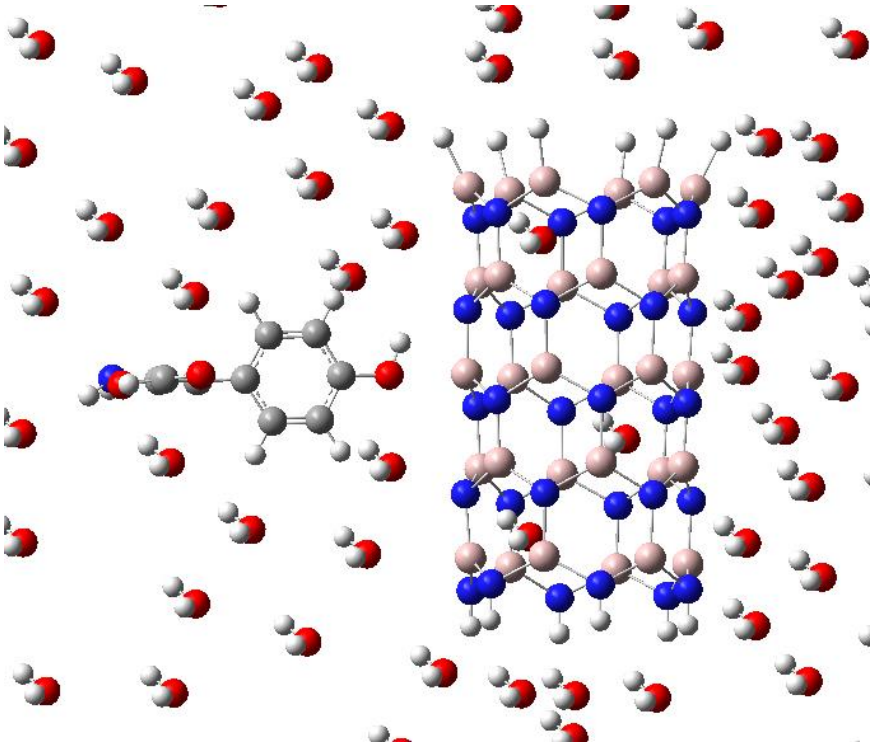


Fig. 4. Interaction of tyrosine with the surface of aluminum nitride nanotube in the direction of alcoholic oxygen on the surface of the aluminum atom in the solvent phase (water).

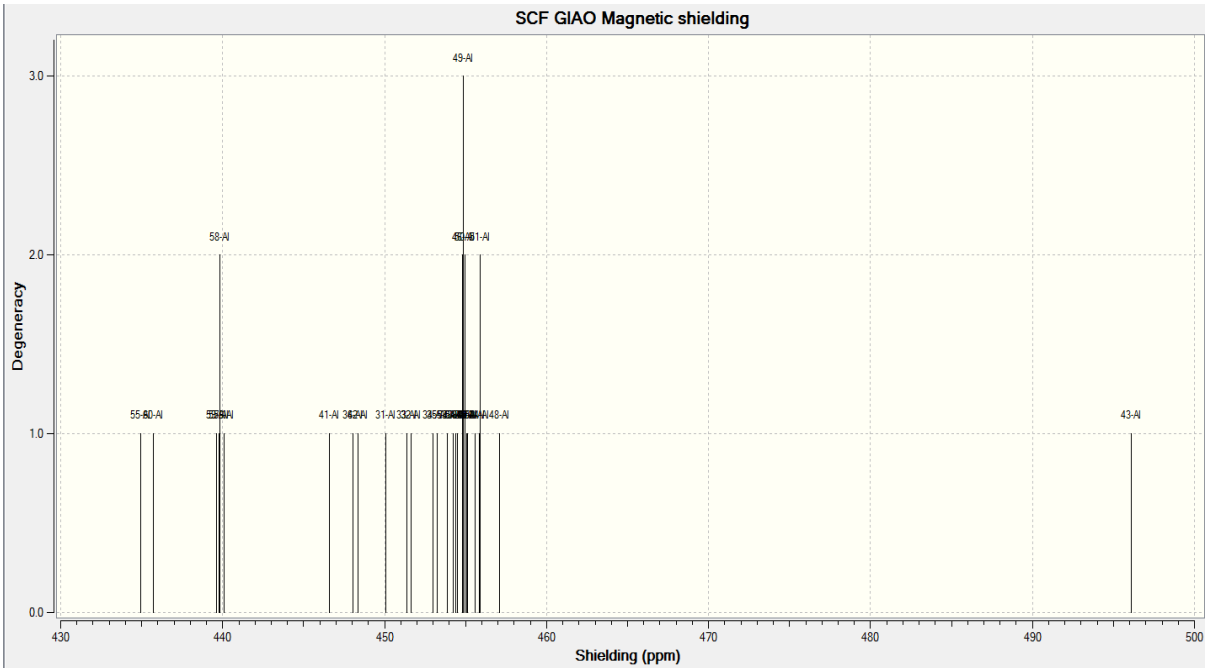


Fig. 5. NMR spectrum of tyrosine molecule adsorption on the surface of aluminum nitride nanotube in gas phase.

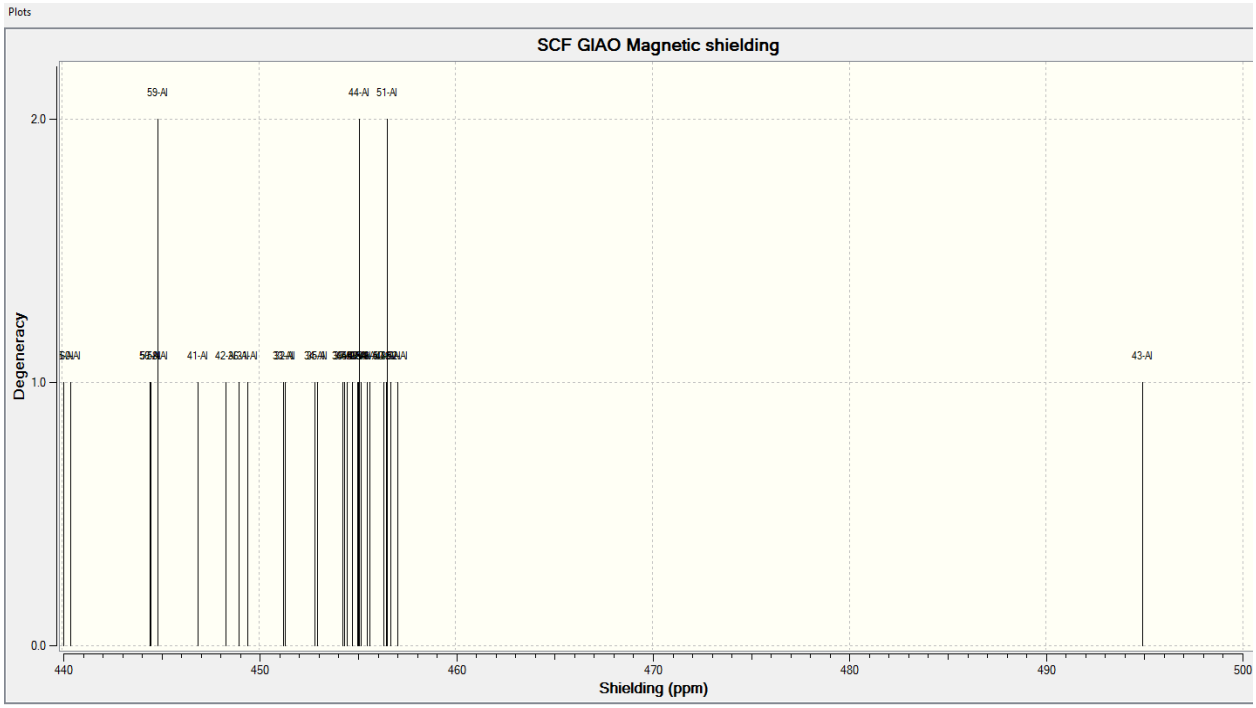


Fig. 6. NMR spectrum of tyrosine molecule adsorption on the surface of aluminum nitride nanotubes in the solvent phase.

RESULTS AND DISCUSSION

Hardness indicates the increase or decrease of the chemical potential of electrons and plays an important role in the theory of electronic structure and activity of molecules and is related to the mobility of electrons in a molecular network. Hardness is also known as a criterion for determining and measuring the stability of chemical systems. This quantity depends on the amount of charge, size and polarization and was first defined by two researchers named Parr and Pearson considering the density function. Chemical hardness (h) is defined according to the following formula:

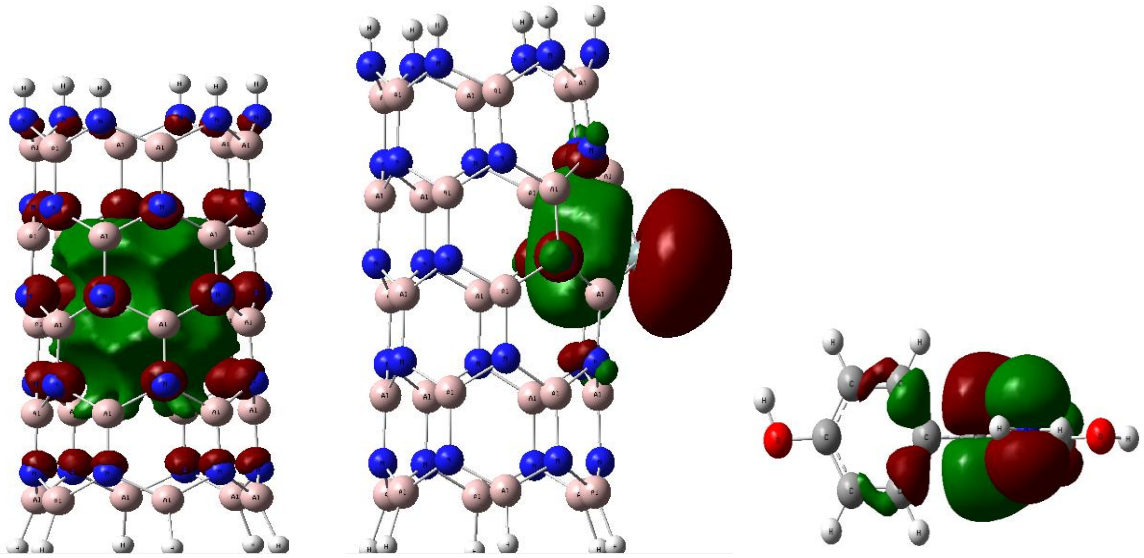
$$\eta = \frac{1}{2}\left[\frac{\partial^2 E}{\partial N^2}\right]_{v(r)} = \frac{1}{2}\left[\frac{\partial \mu}{\partial N}\right]_{v(r)}$$

According to the formula E, the electron energy is a chemical system and N is the number of electrons and V is the external constant potential and μ is the chemical potential. In the non-chemical curve, hardness is the resistance to change. Structures that are stable typically have larger HOMO-LUMO energy gaps and are therefore less active than structures with smaller HOMO-LUMO energy gaps, which require maximum hardness.

The results of the calculated energy level for the structure of tyrosine alone are observed with the base series 3-21G, 6-31G, 6-31G *)). These values show that the resulting values for the energy of the structure under study at the optimal level of the different computational series are almost identical. The same is true for the bipolar torque. Structures depend on their electrical conductivity, which the shorter the distance, the better the electrical conductivity, and conversely, if the distance is large, the electrical conductivity will be intermittent. The results show that the presence of solvent in the calculated energy values and LUMO HOMO levels for the structure of tyrosine alone in the aqueous phase alone was not very

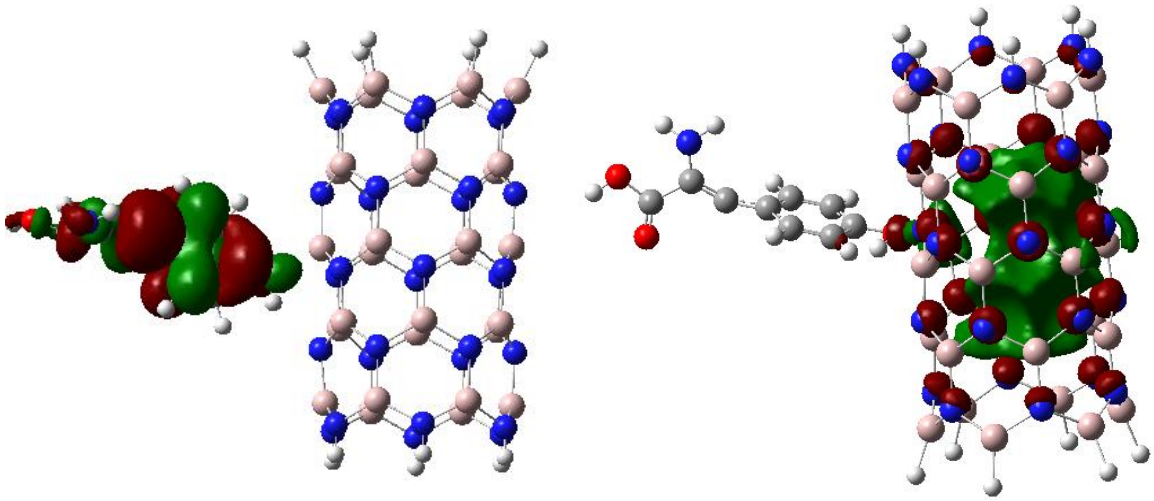
effective, while the values of bipolar momentum underwent more changes.

NMR calculation was performed to achieve the values of magnetic attenuation and chemical displacement in order to calculate the interaction energy. In electromagnetic terms, an isotropic field is one where there is a uniform density or a spherically symmetrical distribution, and the anisotropic field is non-isotropic or non-uniform. Is from the solvent phase.



(a) (b) (c)

Fig. 7.a) LUMO, HOMO aluminum nanotube - nitride b) aluminum nitride nanotube hybridized with silica atom c) tyrosine molecule.



(a) (b)

Fig. 8.a) LUMO HOMO, surface tyrosine adsorption b) aluminum nitride nanotube hybridized with silica atom.

The results showed that the bond lengths of aluminum nitride nanotubes decreased slightly after adsorption, which indicates that the adsorption of tyrosine was poor, but in silica atom aluminum nitride nanotubes, these changes were significant compared to the state of pure nanotubes. Therefore, based on the changes in the bond length of the nanotube due to the interaction with the tyrosine molecule, we can say that the appearance of silica has caused more adsorption of tyrosine.

As we know, a silica atom has an empty orbital in its capacitance layer and is an electron acceptor. Oxygen and nitrogen atoms have electron pairs, so they are electron donors. The results show that the silica atom has a positive charge, which accepts electron pairs, the oxygen and nitrogen atoms have a negative electric charge, in other words, the electron pair. According to the results of the electric charge of aluminum nitride nanotubes (6, 0) in the presence of silica atoms is more negative than aluminum nitride nanotubes (6, 0) without silica atoms. When a tyrosine molecule is added without the presence of a silica atom because it has an electron pair, then the total electric charge of the aluminum nitride Q (C) nanotube is negative, and so is the configuration of the aluminum nitride nanotube (6, 0) in the presence of the silica atom. Because we have silica atoms in nanotubes (6, 0) the total electric charge of aluminum nitride nanotubes (6, 0) is negative. But in other configurations, such as the silica atom and the tyrosine molecule in the nanotube (6, 0), the tyrosine molecule provides its electron pair to the silica atom. Therefore, the total electric charge Q (C) for aluminum nitride nanotubes (6, 0) is zero.

CONCLUSION

In this research, using quantum calculations based on the theory of surface adsorption density of tyrosine molecule on the outer wall of aluminum-nitride nanotubes (6 , 0) as well as aluminum-nitride nanotubes (6 , 0) in the presence of silica atoms were studied. (6, 0) and tyrosine were first optimized by B3lyp method and 6-31 G (d) base and its structural and electronic parameters were extracted. Then, by connecting the silica atoms, the new nanotube structures were optimized again. The results of various calculations show that the total electron energy in the aluminum-nitride nanotubes (6, 0) and the tyrosine molecule are more stable for all configurations in the presence of silica atoms and the surface adsorption of aluminum nanotubes. Nitride is a type of physical adsorption. Chemical hardness calculations for aluminum-nitride nanotubes showed that aluminum-nitride nanotubes (6, 0) and tyrosine molecule have the lowest chemical hardness in the presence of silica atoms. (6, 0) and the tyrosine molecule is larger in the presence of silica atoms. Therefore, it is more soluble in a polarized solution. Comparing the changes in bond length in the interaction of tyrosine molecule at the surface of aluminum-nitride nanotubes and aluminum-nitride nanotubes seen with silica atoms, we can say that due to the small changes that occur during the bonds of tyrosine molecules and nanotubes, as well as changes in their angle (Both tyrosine molecule and nanotubes) This molecule can be better transported by the surface of nanotubes seen with silica atoms. The density of the charge on the surface of the nanotube seen with the silica atom is higher. The higher the density of the electric charge, the better the tyrosine molecule is absorbed. NBO analysis shows that the stability energy for aluminum-nitride nanotubes (6, 0) and tyrosine molecule is higher in the presence of silica atoms. Due to the stability of the structures, aluminum-nitride nanotubes (6,

0) can be used in the presence of silica atoms as a suitable substrate for molecule transfer.

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بررسی جذب تیروزین روی سطح آلومینیوم تک جداره - نیترید و آلومینیم – نیترید - سیلیکون دوپ شده

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چکیده

در این تحقیق رفتار جذب یک مولکول تیروزین روی سطح خارجی نانولوله آلومینیوم نیترید و آلومینیوم-نیترید رویت شده با یک اتم سیلیس با استفاده از نظریه تئوری تابعیت چگالی (DFT) مورد بررسی قرار گرفته است.از پارامترهای محاسبه شده در این تحقیق انرژی بهینه شده، NMR، NBO تغییرات طول پیوند در فاز گازی و حلال را می‌توان بیان نمود.انرژی پیوندی نشان می‌دهد که جذب این مولکول بر روی نانو لوله آلومینیوم نیترید هیبرید شده با اتم سیلیس بهتر از نانولوله آلومینیوم نیترید خالص می باشد و با توجه به نتایج NBO،NMR این نتیجه را می توان اثبات کرد. نرم افزارهای بکار رفته در این محاسبات نرم افزارهای گوس ویو، گوسین می باشند. براساس نتایج بدست آمده از نانولوله آلومینیوم نیترید رویت شده با اتم سیلیس می‌توان در انتقال مولکول تیروزین استفاده نمود انرژی بدست آمده برای انتقال مولکول تیروزین بوسیله نانولوله آلومینیوم نیترید ۹۵۵٤/۰٦۱۷- هارتری و انرژی انتقال مولکول بوسیله نانو لوله آلومینیوم-نیترید رویت شده با اتم سیلیس ۹۵۵٤/۱۲۳- هارتری می‌باشد.

کلید واژه‌ها: جذب سطحی؛ نانولوله‌های آلومینیوم نیترید؛ داروی تیروسین؛ تیوری تابع چگالی

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