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Chemical design of boron-nitride nanotubes, nanotubes by Gaussian 5.0 version

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Abstract
In this study, nano tube modular is utilized to create a graphene nano-ribbon structure with n=m=4 and a tube length of 1 nm. For the display system, export the structure to the Gaussian 5.0 version. The input data is then exported to Gaussian 09, which is used to calculate geometrical and electrical parameters, as well as adsorption energy. The ground state parameters were computed using the DFT approach, which was dependent on electron density. Higher Occupied Molecular Orbitals (HOMO) and Lower Unoccupied Molecular Orbitals (LUMO) are produced by molecular orbital energy, and the energy gap.

Keywords: Gaussian 5.0 version**,** nanotube**,** Boron-nitride nanotubes

Introduction
In all the relevant references, we find that the word nano is a Greek word meaning dwarf, which can be It literally means 'nano technology' describes everything small and precise hence the term And if we use the word nano to describe all the minute particles, and in this case the finite particles In childhood, we can describe this technology as 'Nanotechnology', [1]. This word is in order to know the true meaning of it. The word nano means one part of a billion part of any 10 of something, and scientifically we find that the word nano means one part of a billion part of something, and in the language of numbers 9 meter, and this means that when we divide one linear meter into one billion parts, one part of these that parts represent one nanometer, and to approximate the image more, [2] let's take one human hair for a minute, Thickness After looking at the small diameter and accuracy, let us suppose that the width of the diameter of this hair is 80 micrometers, so if we divide this minute hair into 80,000 times, that is, we divide it into 80,000 divisions. The thickness of one of these sections is equivalent to one nanometer [3, 4]. And to approximate the meaning, the size of the nano About 80,000 times smaller than the diameter of a human hair, and the smallest thing that a human can see With the naked eye, it is about 10,000 nanometers wide, and when ten atoms of Hydrogen for hydrogen has a length of one nanometer [5]. This length is close to the length of viruses DNA, atom diameter, and nanotechnology specialize in dealing with all these things, the most important of which are [6] In which is clarification 1-I Atom and DNA. And for more clarity, let us study the figure (1). The levels of the scales of things, which were divided into three levels “the millimeter level” and “the millimeter level” micrometer" and "nanometer level", [7] and this figure also shows the means of seeing things, which are divided and in general, there are three methods: "the naked eye and microscopes" and "micron microscopes" and " nanometer microscopes.” The figure (1) also shows the physical laws that govern and describe the world of these things. We find that there are two types of physics, classical physics which deals with the big world and which ends [8]. Its limits are by approaching the level of nanoparticles, and quantum physics, which deals with the exact world, which it starts from the world of nanoparticles and extends to the world of atoms and nuclei and beyond [8]. We find some fine particles, through which it is possible to approximate the image of nano dimensions. For example, we find-I and in Fig (1). 5000 and the average length of 2000 nm to 2000 nm that the length of red blood cells in humans ranges between 2.5 As for one nanometer, it is equivalent to the distance occupied by ten atoms nm. It is about a DNA molecule [9] hydrogen side by sid

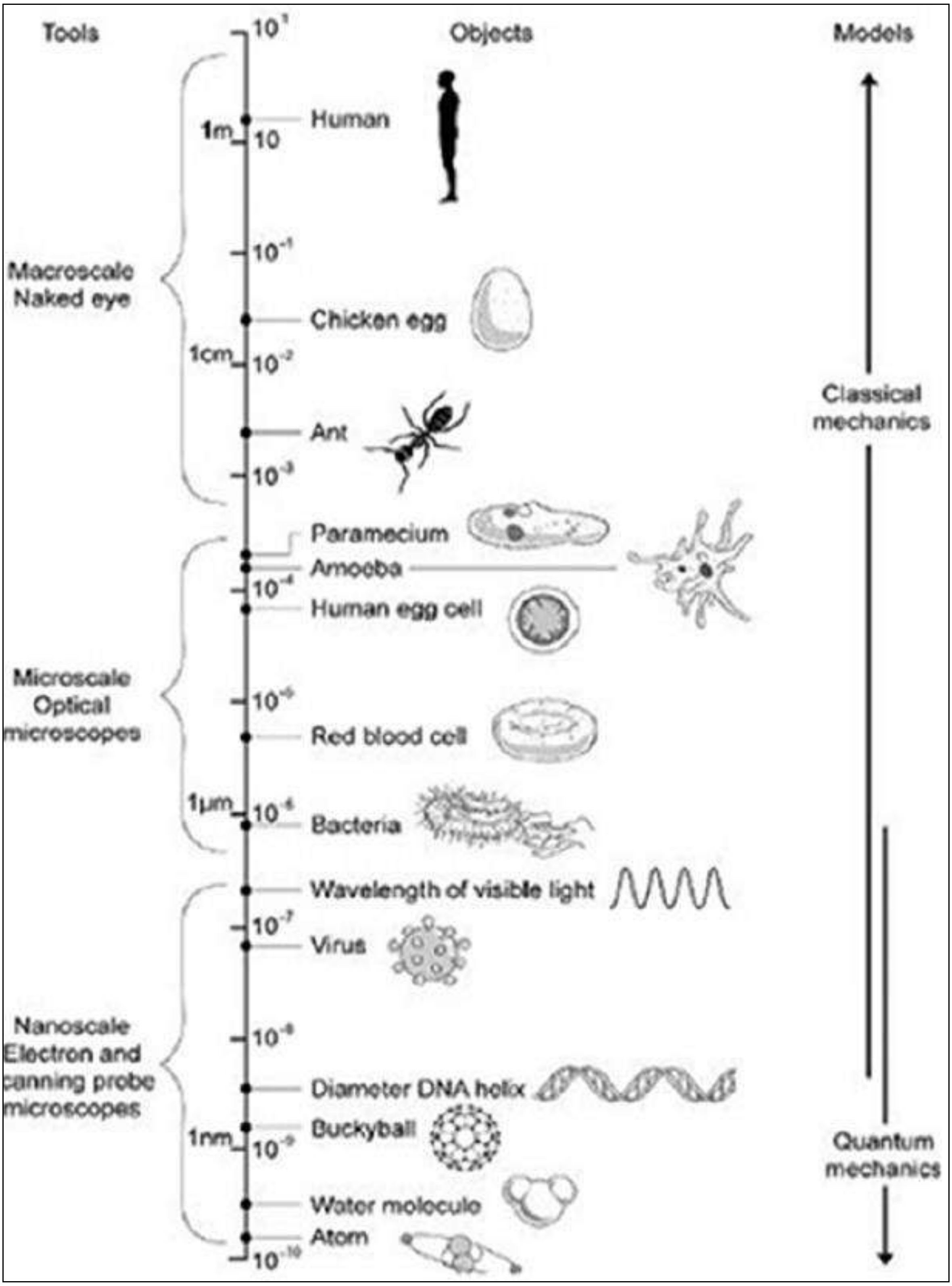

Fig 1: Means, tools, materials and physical laws applied in different dimensions

By using nanotechnology, the physical, biological and chemical properties can be combined. The employment of materials is possible in any field, whether the human body, or in the engine of an aircraft Putting the atoms involved in the handling in a specific way, so the resulting materials will be more accurate [10]. It is more pure than traditional manufacturing, and it is the result of standardizing the quality of the product, as well as reducing the cost of production and Reducing the energy consumed, there are devices at the nano level Able to direct atoms (Nanodevice) reduce the energy consumed, there are devices at the nano level 2-I and put it in its correct place during the reaction process shown in Figure (2) [11].

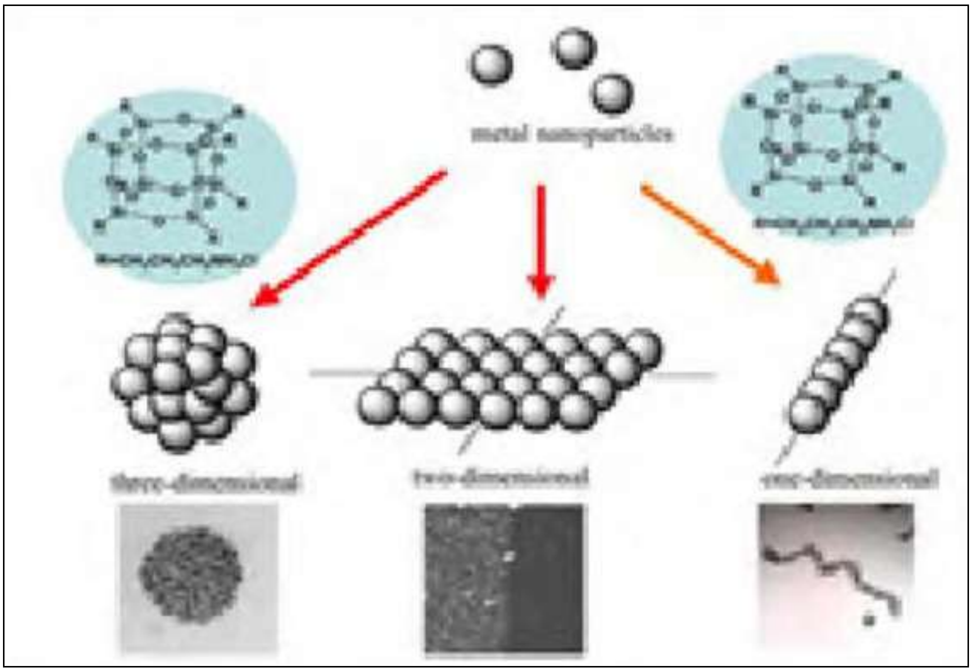

Fig 2: How are the atoms oriented during the reaction

Distinguishing properties of nanoparticles I that there are many physical, chemical and mechanical properties that distinguish nanoparticles from Larger particles and materials, and by largest, we mean any particles whose dimensions are greater than 100 nanometers, [12] and We can know these larger particles as particles of ordinary dimensions, that is, in their state And in this case are the particles whose dimensions are greater than 100 nanometers, where the large (bulk materials) We find that when materials are nanoparticles (their dimensions are less than 100 nanometers), they appear and give completely different and different properties from its properties when it was in its normal state and these properties And this phenomenon made nanoparticles a “new scientific miracle” [13]. You can imagine that the properties. What is known to us about a material will be completely different when this material is a nanoparticle, for example, insulating materials. They become conductors when they become nanoparticles, and conductors become insulators when they become particles Nano, and so many and many other impressive behaviors and characteristics, but here we will quickly refer to some these characteristics. One of the distinguishing properties of nanoparticles [14] is the ability to change color when it changes color. The size and shapes of these particles, and this phenomenon is found in some elements such as gold, as well as .The element of silver, in addition to their golden and silver colors that are well known to us, we find that the color of the gold solution It changes from golden to orange suddenly when its particle size is less than 100 nanometers, [15] and the color of this solution becomes green when the size of the gold particles is less than 50 nanometers As for the silver solution, its color changes (nano-spheres), noting that the gold particles are spherical in shape. About 100 (nano-prisms) silver suddenly turns red when its pyramid-shaped particles decrease in size nanometers, but if we have a solution of silver particles of spherical shape, the colors of this solution change. To light yellow when the particle size is less than 120 nm and to light blue when [16]. The particle size is less than 80 nm and also to dark blue color when the size is reduced 4- I-particles about 40 nm (see Figure 3).

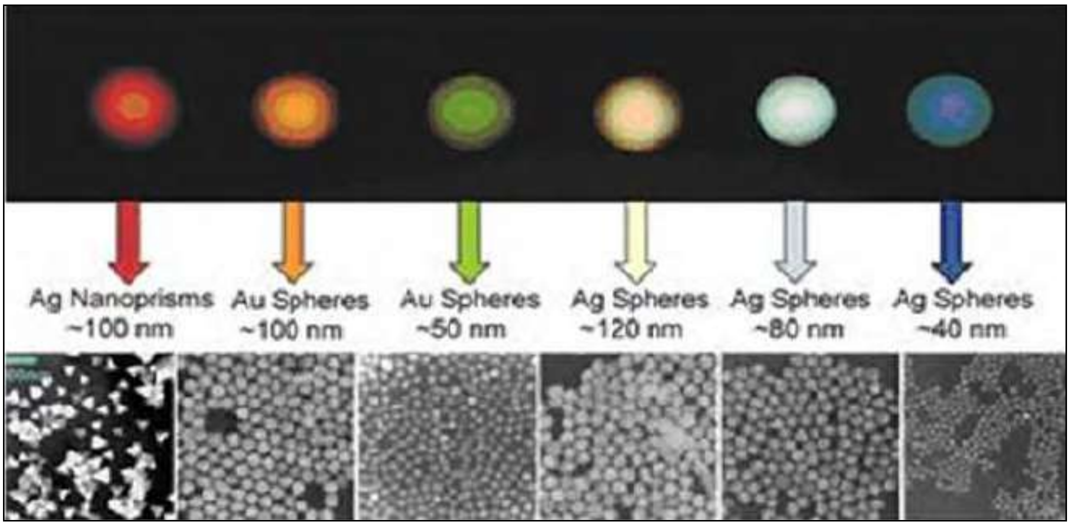

Fig 3: Change the color of the gold nanoparticles solution

One of the unusual properties of nanoparticles is also the property of hardness, where we find that the hardness of nanoparticles .Nanoparticles of a substance are hundreds of times greater than their hardness in their bulk state [17]. And (silicon nano-spheres) experimentally that the hardness of spherical nanoparticles manufactured from silicon. Its size ranges from 40 nanometers to 100 nanometers, hundreds of times greater than the hardness of silicon. It has a hardness that makes it one of the hardest materials on earth, and in particular it has a hardness between hardness Sapphire and diamond. Also, the property of transparency is the property of the nanoparticles with dimensions less than the lengths [18]. Therefore, it does not reflect or refract light, which makes it highly transparent, which means that it can be used in many applications without affecting the color or shape of the product as it is.

Result

1. Carbon nanotubes

In this study, nano tube modular is utilized to create a graphene nano-ribbon structure with n=m=4 and a tube length of 1 nm. For the display system, export the structure to the Gaussian 5.0 version. The input data is then exported to Gaussian 09, which is used to calculate geometrical and electrical parameters, as well as adsorption energy. The ground state parameters were computed using the DFT approach, which was dependent on electron density. Higher Occupied Molecular Orbitals (HOMO) and Lower Unoccupied Molecular Orbitals (LUMO) are produced by molecular orbital energy, and the energy gap [19].

The geometrical properties of SWCNT at ground state are evaluated using DFT calculations in this study. Figure 1 depicts the geometrical structure of SWCNT, which includes bond length and angle between atoms that produced it. The outcome of the figure reveals that there are four types of bonds between atoms that are related to SWCNT. The lengths of their (C-C, C=C, C—-C, C-H) bonds are (1.4566-1.4801, 1.3546, 1.1413-1.4421, and 1.0853), [20] respectively. The lengths of the C=C and C-H bonds are symmetric in values, according to the results. The angles between atoms (C-C-C, C-C—-C, and C-H=C) are (119.1111-119.1280, 115.5075-120.5344, and 121.8984-121.9001). All of the bond length and angle results correspond with those found in an earlier study.

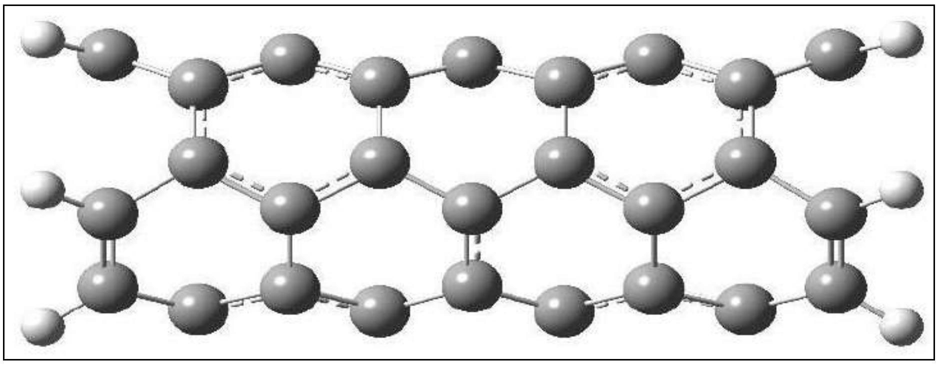

Fig 4: Structure of SWCNT, the white and gray balls are H and C atoms, respectively

The energy gap and molecular orbitals are effective tools for characterizing the amount of charge transportation between band energies. DFT simulations are used to investigate the properties in question 1. Table 2 shows the electronic states (HOMO and LUMO) as well as the energy gap in eV units. Results shows that SWCNT was semiconductors materials.

2. Boron-nitride nanotubes

BNNT was used in present study has chirality (4, 4) and tube length is 1 nm zigzag edge. The BNNT geometry structure is displayed in Figure 1a. For the boron-nitride ribbon the bond length between B-N, (N-H) and (B-H) are (1.4539), (1.0121) and (1.1909) Å. Angles between atoms N-B-N and B-N-B are (119.9977) and (120.0011) degree, the result shows that agreement with a previous study.

Table 1: Represent values of electronic states (HOMO and LUMO) and energy gap measured in eV unit

System	HOMO	LUMO	Eg
SWCNT	-4.5594	-2.3006	2.258

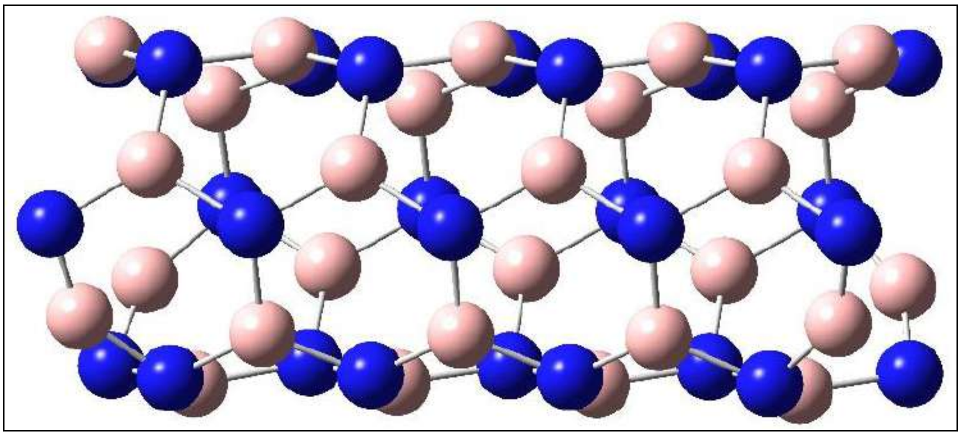

Fig 5: Represent values of electronic states (HOMO and LUMO) and energy gap measured in eV unit

Energy gap consider one of the important factor that pointed nature of materials (conductors, semi-conductors and insulators) depending on change in molecular orbitals energy. The HOMO and LUMO energies were about -7.302 and -1.974 eV; respectively, the energy gap was 5.327 eV. The result shows that BNNT has an insulator nature because it has wide band gap energy.

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