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Precise Atomic Structures of Three Novel Nanomaterials in Nanotechnology, Biomedicine and Cosmology: Graphene, Boron Nitride and Coronene

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INTRODUCTION. Nanomaterials are currently of great importance in science, technology and commercial applications [1,2]. Since these materials are atomic layer thick and are a few square nanometers of area, a knowledge of their precise atomic structures will help in the exact understanding of the properties at the nanoscale and in the fabrication and design of the nanomaterials for their many uses. Their known inter-atomic distances have been used here to obtain the exact atomic radii of the component atoms and thereby their precise atomic structures, *for the first time*. Considered here are three nanomaterials with hexagonal structures, but of quite different properties, namely, graphene (an electrical conductor), boron nitride (an insulator) and coronene (indicators of life in the Universe).

GRAPHENE: $(C_6)_n$

"WHAT IS GRAPHENE?"

- **GRAPHENE** is an inorganic material consisting purely of carbon atoms bonded together as regular hexagons in a 2-dimensional sheet, see Fig. 1, [3].
- **GRAPHENE** layers are bound by van der Waals forces in 3-dimensional graphite, see Fig. 2, [4].
- **GRAPHENE** is the basic building block of many important nano-materials, like fullerenes, carbon nanotubes, etc, see Figs.3 & 4, [5,6].

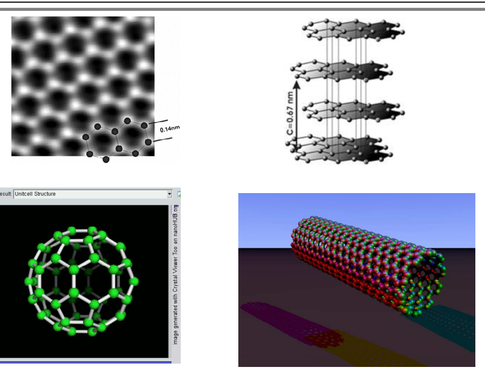


Fig. 1. (Top left): Graphene, as seen by transmission electron microscope.
Fig. 2 (Top right): Graphite (graphene layers bonded by van der Waals' forces)
Fig . 3 (Bottom left): Fullerene (graphene curled up).
Fig. 4 (Bottom right): Carbon nano-tube (graphene rolled up).

"VERY EXPENSIVE MATERIAL ON EARTH"

- Although it is formed by as simple a process as scratching a pencil on a paper, graphene produced by exfoliation, with a sample the size of the cross section of a human hair costs [3] more than

"$1,000 (as of April 2008) which is about $100 million/cm^2"

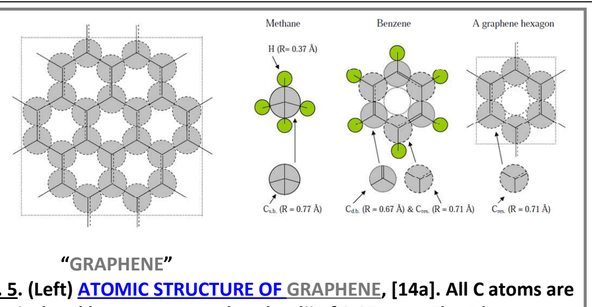
- However, procedures are being developed to bring down the price.

"IMMENSE USES AS A NANO-MATERIAL"

- It is chemically inert, electrically conducting and optically transparent.
- Hence its immense potentialities for applications in various fields of nanoscience and technologies. See e.g., [7,8]. To mention just a few:
- Graphene as LCD in computers, TV, cell phones, [9], high speed optical communcation [10], solar cells [11]
- Graphene in biomedicine as biosensors, and for disease/toxin detection as nano-structures with DNA [12,13]

"PRESENTED BELOW, IS THE PRECISE ATOMIC STRUCTURE OF GRAPHENE"

- The known carbon-carbon bond distance of 0.142 nm [3] in graphene is the sum of the radii of two similar carbon atoms of resonance bond radii = 0.071 nm [14a], see Fig.5.
- The electrical conductivity of graphene is due to these resonance bonds [14b].
- Fig. 5 shows how seven graphene regular hexagons are contained in an area of ~0.9 x 0.9 nm (= 0.8 nm^2 < 1 nm^2).
- With this exact knowledge of the atomic geometry, one can now understand its properties better and design the materials more exactly for use in nanotechnology, biomedicine and commercial applications.



"GRAPHENE"

Fig. 5. (Left) ATOMIC STRUCTURE OF GRAPHENE, [14a]. All C atoms are identical and have resonance bond radii of 0.071 nm. The 7 hexagons with 24 C atoms occupy an area of 0.9 x 0.9 nm (= 0.8 nm^2).
Fig. 6. (Right): Methane, (C has covalent single bond radius of 0.077nm as in diamond), Benzene with bond length, 0.138 nm (accounted by 3 C atoms with covalent double bond radii of 0.067nm and 3 with resonance bond radii of 0.071 nm as in graphene), and Graphene (unlike in benzene all C atoms have equal radii, 0.071 nm), see [14].

BORON NITRIDE, $(B_3N_3)_n$

WHAT IS BORON NITRIDE?

- **BORON NITRIDE,** is an inorganic chemical compound with equal number of boron and nitrogen atoms. It forms a hexagonal layer structure like graphene, and stacks at distances of about 0.33nm like graphite (and hence also called as white graphite), see Fig. 7, [15].
- **BORON NITRIDE** forms nanotubes like carbon nanotubes, see Fig. 8, [16] and also forms nano-mesh of very interesting properties and applications [17].

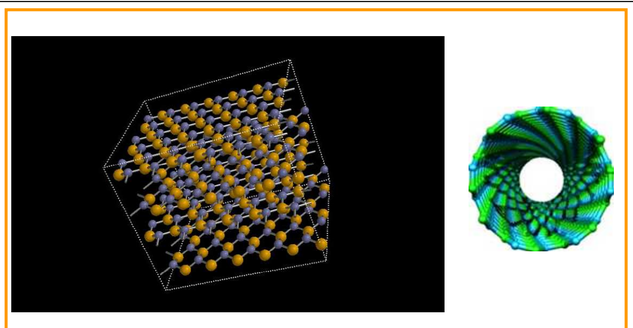


Fig. 7. Boron nitride layer lattice (bound by vdW forces at distances of 0.33 nm) [15c] (left).
Fig. 8. Boron nitride nanotube [16a] (right)

"THIS IS ALSO AN EXPENSIVE MATERIAL

- It is not found in natural form, but is synthesized from boric acid and boron trioxide. The amorphous form so obtained is heated to a high temperature in nitrogen to obtain the crystalline form [15,18].
- It is expensive, but less so than graphene, costing [19] about $100 per pound!
- Cost of nanosheet (obviously higher)

"HAS NUMEROUS USEFUL PROPERTIES"

- Excellent thermal and chemical stability: BN ceramics are traditionally used as parts of high-temperature equipments [19,20].
- Has excellent lubricating properties and is used as additive to cosmetic products, dental inserts and in space equipment. In the hot pressed state, h-BN is readily machinable [19,20].
- Not wetted by most molten metals, glasses and salts and hence has a high resistance to chemical attack [21].
- Is an electrical insulator, making it an immensely useful technological and commercial insulating material [19,21].
- BN nanotubes have been used in the study of living cells in bio nanomedicine [16b,22,23]. For more uses of BN in biomedicine see [16,23]
- BN nanomesh is a new inorganic nanostructured material, [17,24]
- Is very stable under vacuum, air and some liquids and at high temperatures. It shows extraordinary ability to trap molecules and metallic clusters. The nanomesh has applications in nanocatalysis, surface functionalisation, spintronics, quantum computing and data storage media like hard drives [25].

"PRESENTED BELOW, IS THE PRECISE ATOMIC STRUCTURE OF BORON NITRIDE"

- The known boron-nitrogen bond distance of 0.145 nm [26] is the sum the covalent single bond radii of the boron and nitrogen atoms of 0.075nm and 0.070 nm [27] resply., (see Fig.9), [14c].
- Fig. 9 shows how seven boron nitride regular hexagons are contained in the small frame of area of ~0.9 x 0.9 nm (= 0.8 nm^2 < 1 nm^2).
- With this exact knowledge of the atomic geometry, one can now understand its properties better and design the materials more exactly for use in nanotechnology, biomedicine and commercial applications.

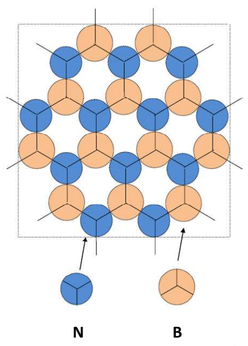


Fig. 9. ATOMIC STRUCTURE OF BORON NITRIDE, (h-BN), [14c]. The hexagons consist of equal number of B (copper color) and N (blue) atoms with bond length d(BN) = 0.145 nm and radii d($N_{s.b.}$) = 0.070 nm, d($B_{s.b.}$) = d(BN) – d($N_{s.b.}$) = 0.145 – 0.070 = 0.075 nm.

CORONENE, $(C_{24}H_{12})$

WHAT IS CORONENE?

- **CORONENE** is an organic compound. It is a highly symmetrical polycyclic aromatic hydrocarbon (PAH) consisting of a "flat" ring of six fused benzene (C_6H_6) molecules, colloquially known as super-benzene, see Fig 10, [28,29].
- **CORONENE** is an aromatic compound consisting of carbon and hydrogen atoms, whereas graphene consists of hexagons of *only* carbon atoms.
- **CORONENE** crystals are parallel stacks of layers of the PAH held at the inter-layer distances of about 0.35 nm by van der Waals forces, as in graphite.

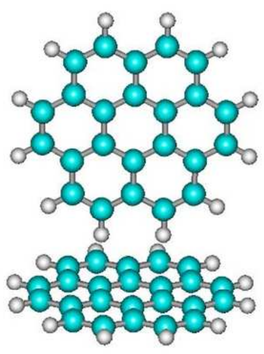


Fig. 10. Coronene (model) [29a].

"THIS IS A VERY EXPENSIVE MATERIAL"

- **CORONENE** occurs naturally as the mineral carpathite, which forms flakes in sedimentary rocks. The molecules are also found in the interstellar medium, in comets, and in meteorites and are candidate molecules to act as a basis for the earliest forms of life, [28,30].
- **CORONENE** is an expensive compound and it costs [31] about 1800 Euros per gm!
- Cost of nanosheet (obviously higher)

"HAS NUMEROUS USEFUL PROPERTIES"

- **CORONENE** is a yellow substance which fluoresces blue under ultraviolet. It also forms nanotubes [28,32].
- Its intriguing structure and vibrational activity are now attracting interest from astronomers as potential indicators of organic life elsewhere in the universe [28,30,33,34].
- It is also of interest to materials scientists who see it as the smallest possible unit of nanomaterials, which are now being keenly researched as future molecular scale electronics components [34].
- However, superaromatic coronene remains enigmatic in some ways to the organic chemists. The molecular structure and vibrational motion of the aromatic hydrocarbons still pose considerable theoretical challenges [28,34].
- **CORONENE** too has biomedical applications [35,36].

"PRESENTED BELOW IS THE PRECISE ATOMIC STRUCTURE OF CORONENE"

- The CC bond distance of 0.138 nm in coronene, as in benzene [14a,29b], is the sum of the radius of one C atom with covalent double bond radius (0.067nm) and one with resonance bond radius (0.071nm) (as in graphene).
- Fig. 11 shows the coronene molecule [14c]. The 7 regular hexagons are contained in the small area of ~0.85 x 0.83 nm (= 0.7 nm^2). On including the H-atoms, the area is ~ 0.8 nm^2 < 1 nm^2.
- With this exact knowledge of the atomic geometry, one can now understand its properties better and design the materials more exactly for use in nanotechnology, biomedicine and commercial applications.

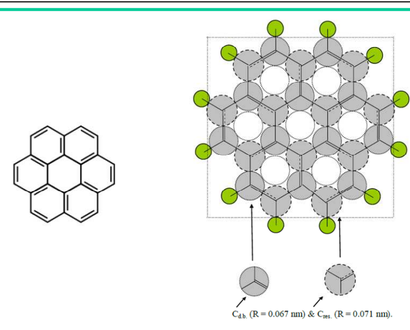


Fig. 11. (Right) ATOMIC STRUCTURE OF CORONENE: [14c]. Consists of six benzene rings fused together. Each benzene ring consists of 3 $C_{d.b}$ atoms with covalent double bond radii (0.067 nm) and 3 C_{res} atoms with resonance (graphitic) bond radii (0.071 nm). Bond distance, d(CC) = 0.138 nm. (Left): Conventional structure of coronene [37].

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REFERENCES: Please see the adjoining sheets.