Egypt. J. Chem. **Vol. 63,** No. 12 pp. 4777 - 4787 (2020)

Egyptian Journal of Chemistry

http://ejchem.journals.ekb.eg/

Molecular Modelling Applied for Carbon Nano Materials

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Abstract

Molecular modelling is applying computer software to describe the molecular systems. This leads to understating many systems and structures in chemical, biological systems. Molecular modelling is now widely used in much basic as well as applied science. On the other hand, carbonaceous materials which also known as carbon nano materials have attracted interests of many researchers according to their amazing special structures and extraordinary electronic properties. So that, research on the carbon nano materials are now increasing rapidly. Accordingly, carbon nano materials are surveyed with special care to fullerene, carbon nanotubes and graphene as well as their based systems. The review include how can molecular modelling describe the physical, chemical and functionality of the carbon nano materials. The review includes the following points

1. Introduction
2. Molecular modelling
3. Calculated parameters through molecular modelling
4. Carbon nano materials
5. Fullerene based systems
6. CNT based systems
7. Graphene based systems
8. Modelling other forms of carbon
9. Conclusion and outlook

Keywords: Molecular modelling ; fullerene; CNT; graphene..

1. Introduction

Nanotechnology is worldwide science and technology find its applications in all fields, in all fields one can find nanoscale, nanoparticle, nanophase, nanocrystal, or nanomachine. So that, this field attracts worldwide attention. Simply nano scale materials are those with dimension in nano meters which is length scale, in this sense 1 nm is equal to a billionth of a meter (10^{-9} m) [1].

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Receive Date: 29 March 2020, Revise Date: 19 April 2020, Accept Date: 12 July 2020

DOI: 10.21608/EJCHEM.2020.26861.2551

This class of materials is something between chemical interactions which took place among atoms and within molecules in rang below 1 nm and condensed matter physics which is representing clusters of materials gathered in crystals contains huge numbers of atoms. This makes several scientists ranging materials between 1 nm to 100 nm not within chemistry or solid-state Physics. This in turn requires new concepts and design of equipment's to follow up this new branch also requires approximations of the theoretical methods to follow up changes in this nano scale materials. Better understanding of this range leads to continuous developments and achievements in many areas whereas nano materials are applied. It could be here stated that, nanotechnology is the manipulation of matter with at least one dimension sized from 1 to 100 nanometers [2,3].

It is worth to mention that for manipulation of nano scale materials molecular modelling is a promising field. Moreover, carbon nano materials are an important class of nano materials due to its novelty applications in many areas. Accordingly, an introduction to molecular modelling is presented then carbon nano materials will be survived with the focus to their possible studies with molecular modelling .

2. Molecular modelling:

Molecular modelling is simulation conducted for molecular systems to understand the molecular behaviour. It is a class of computational work based on the quantum mechanics designed to study the chemical structures. It is an effective tool in materials science, physics and chemistry. It could be applied whereas experimental facilities are limited or unavailable or ethically not allowed for many systems such as biological systems [4-9]. It computes the energy of a particular molecular system, which leads to predict geometrical parameters; thermochemical parameters and vibrational frequencies including Infrared and Raman beside many other physical as well as chemical important parameters.

Such class of computational work pointed toward enhance the communication between experimental and theoretical research on both existing and new advanced findings based on their amazing applications. It is now worldwide applied for many systems and molecules covering many areas of both basic and applied science [10-14].

Recent applications of molecular modelling are guiding researchers to elucidate the molecular structure and chemical interactions of molecules in many areas of applied research [15-17].

Molecular modelling consists of molecular mechanics and electronic structure method [18], both could be summarized as in the following:

Molecular mechanics: It applies the laws of classical physics to predict the structures and the properties of the molecules. It performs computations based upon the interaction among the nuclei. Electronic effects are approximated, this makes the computations quite inexpensive, and used for very large system.

Electronic structure method: It applies schroedinger wave equation. Practically exact solution of schroedinger equation is not enough so, electronic structure method has many approximations to its solution. It has the following classes

Semi-empirical methods

Ab initio

Density functional methods.

More details about the basic principles of such classes of electronic structure methods were reported [18-20].

3. Calculated parameters through molecular modelling :

For electronic structure method and from theoretical point of view the model is an approximation to solve schroedinger wave equation. So, the model is a theoretical method with basis set.

As stated earlier [21] the method could be Ab initio or density functional theory. While the basis set is a mathematical representation of the orbitals. The combination between a theoretical procedure, and a basis set is used to approximate a solution for schroedinger wave equation. As it is a second order equation, it has two solutions. One of the most important parameters, which obtained through the first derivative, is the optimized geometry of the studied structure that predict bond lengths and bond angles of the structure. It localizes the lowest energy molecular structure in close proximity to the specified starting structure. It depends primarily on the gradient of the energy, i.e. it is the first derivative of energy with respect to atomic position. Moreover, through first derivative one can also obtain the total energy and total dipole moment. Otherwise, the second derivative one can obtain

many parameters such as; vibrational frequencies including Raman and Infrared; polarizability; thermochemical parameters. It is worth to mention that these methods or the solutions could be compared with experimental results after so called corrections or scaling. As these methods contain systemic errors which could be corrected be so called scale factor. Only scaled data could be compared with experimental results.

Carbon nano materials:

Carbon-based materials are now widely used for many applications such family include graphite, activated carbon, fullerene, carbon nanotubes, mesoporous carbon, diamond and recently graphene [21].

Figure 1 presents some types of carbon-based materials as graphite, fullerene, Single walled carbon nanotubes, Multiwalled carbon nanotubes, graphene and Diamond respectively.

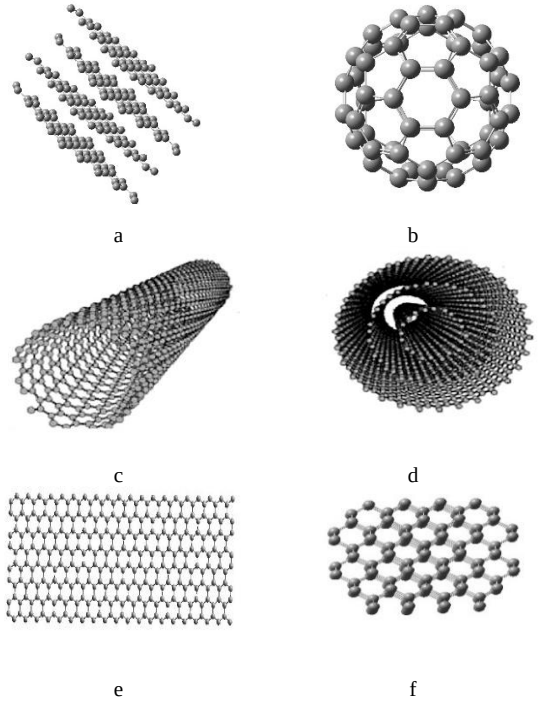

Fig. 1. Carbon based materials a- graphite, b-fullerene, c- Single walled carbon nanotubes, d- Multiwalled carbon nanotubes, e graphene and f- Diamond.

In the following not all but only some members of carbon materials will be surveyed. Starting with fullerene, which is also termed as C_{60} is a member of carbon nano materials since its discovery is considered among the most attractive point of research [22]. Physically, it is described with unusual magnetic properties which may be correlated to its icosahedralv nature. It is corresponding to I_h symmetry, in addition, its magnetic susceptibility arises from the existence of π-electrons ring currents in its carbon spheroid. In 1991, SumioIijima discovered a byproduct of fullerene called carbon nanotubes (CNTs) of two types' single-walled nanotubes and multi-walled nanotubes. Single-walled nanotubes with growing diameters being arranged (like "Russian doll") in a concentric manner, while multi-walled nanotubes may consist of one rolled up graphene sheet [23]. Carbon nanotubes could be produced in considerable amount using catalytic decomposition of acetylene in the presence of supported Co and Fe catalysts [24]. Another method could be achieved by a 60 keVAr^+ ion bombardment with normal incident angle under high vacuum. In such method fullerene was first transformed into amorphous carbon then formed carbon nanotubes [25]. Both fullerene and Carbon nanotubes could be also produced using the conventional catalytic Chemical Vapor Deposition (CVD) with certain care single-walled carbon nanotubes could be also produced [26]. Other modifications for producing could be reported elsewhere [27-29]. Since the discovery of CNTs till now, it attracts interest due to their side range of applications, including high strength [30], extraordinary flexibility [31], excellent electrical conductivity [32] and field emission properties [33], which promise tremendous applications in electron field emitter of displays [34], nanoscale electronic devices [35], biosensors [36], hydrogen storage [37] and fuel cell electrodes [38]. Graphene is a two-dimensional structure; its carbon atoms is considered as surface atoms [39]. This makes its electronic properties is changed with introducing atoms like transition metals and/or metal oxides [40-41] this could be also achieved with molecules as well [42]. When graphene is interacted with metal nanoparticles (Ag, Au, Pt and Pd) there is a significant charge-transfer interaction which dedicates this composite for many applications depending on their surface [43]. Although graphene is a member of carbon nano materials , it is now the parent of a new family of graphene-based materials [44]. Such a new family is not only for gas sorption but also for energy storage [45]. Increasing the applications of modified graphene comes from the fact that graphene properties are not only a function of its number of layers but also a function of the

structural defects [46]. As indicated earlier, such defects could be achieved with doping or decoration, which enhances the ability of graphene to carry out its task. Moreover, it becomes highly sensitive and selective to act as gas sensor. Continuous work on graphene-based materials indicated its suitability to act as electrochemical biosensors for different materials including ascorbic acid; dopamine; uric acid; amino acid tryptophan as well as detecting nitrite in human serum [47].

4. Modelling carbon nano materials :

Applying molecular modelling could be effective tool to investigate different properties of carbon nano materials. In this section it will be directed to three members of the family namely fullerene, carbon nanotubes and graphene.

5. Fullerene Based Systems:

As mentioned earlier fullerene is belonging to structures of ambiguous aromatic character; traditional measurements are not providing proper classification [48]. This in turn paves the way toward new powerful characterizing tools to investigate it. Doping and/or substation could enhance the electronic properties but following up the effect of that could be described on the theoretical basis. Molecular modelling with Mont Carlo simulation level is utilized to calculate the pauli paramagnetic susceptibility of A_3C_{60} (A=K, Rb) compounds [49]. This confirming the findings that, C_{60} is an aromatic molecule with a vanishingly small ring current magnetic susceptibility [50]. Molecular modelling with different level of theories show the ability for calculating important physical and chemical parameters necessary for understanding the properties of fullerene. Quantum mechanical calculations using Ab initio was used to elucidate, the structural and electronic properties of small silicon clusters and endohedral metallofullerenes [51]. Some efforts were also utilized with Density Functional Theory, DFT for reporting the structural parameters then the stability of $C_{60}CH_2$ [52]. Another level of theory at Ab initio was also conducted for studying stability of MC_{60} where M is Sc, Y, and K respectively [53]. The same level of theory was also consulted for describing in details the equilibrium structure of giant fullerenes [54]. Calculations upon inorganic fullerene spheroids were performed at semiempirical molecular orbital calculation. Some important parameters were calculated including geometrical parameters, electronic properties, and then vibrational characteristics [55]. The fullerene family include another members and derivatives, the structure, stability and polymerization of C_{28} was calculated with ab initio quantum mechanical level [56]. Computational levels are also modified in order to follow up the changes in the C_{60} systems. The first-principles DFT calculations were utilized to describe the adsorption of C_{60} on Si (111) [57]. Another computational effort was carried out at Ab initio level to investigate the interaction between C_{60} and Si (100) [58]. Calculation are predicating the stability of other fullerene members so that, it is proven that, g-C_{80} and g-C_{240} cages are less stable and have smaller HOMO–LUMO gaps as compared with their graphite isomers [59]. Time-dependent DFT combined with sum-over-states method were utilized to estimate the static third-order optical susceptibility $\chi(3)$ for BN fullerene materials [60]. Semiempirical calculations were proposed to study the structure and vibrational properties of C_{60}, C_{80} as well as their epoxides [61]. As an application of the effect of doping, it is stated that C_{60} behave like superconductor when it is doped with K [62]. But this requires some kind of cooling around 18k. This paves the way toward C_{60} doping with alkali metals then superconducting properties achieved, including high critical magnetic fields [63]. Further efforts are then emphasis that, the alkali metal doped C_{60} are good candidates for superconductivity based on their unique electronic structure [64]. Based on Ab initio calculations, the phonon spectrum of K_6C_{60} are presented. The effects of doping upon the infrared frequencies and their intensities are identified and correlated with their physical origin. The results are discussed in detail for optically allowed modes [65]. Other efforts were carried out for doping, as a hole doped C_{60} at relatively higher temperature around 52 k [66]. Rather than doping with metals other way of interactions could be achieved with functional groups and/or other chemical organic structures. So that, C_{60} were interacted with $CHCl_3$ and $CHBr_3$ it is reported that an expansion in the lattice took place [67]. According the unique electronic properties of modified fullerene it is also applied as device. It is tested as photovoltaic cells when is prepared in polymeric matrix [68]. Experimental efforts are conducted to prepare filamentary K-C_{60} superconductor by the suspension spinning method.

Results show superconductivity with Tc=18 K, which was indicated by SQUID measurement [69]. This in turn enhances the applications of fullerene composite as polymer photovoltaic cells. Accordingly, conjugated polymer/ C_{60} composite was prepared for this purpose [70].

C_{60} was further mixed with polystyrene then, bistability in single layer devices was observed. This was the first principle toward the applications of such class of materials as devices in disposable printable electronics [71]. According to the amazing properties and applications of composite materials based on C_{60} it is combined with carbon nanotube for many advanced applications including X-ray, neutron as well as high-energy particle physics [72].

6. CNT based systems:

The structure of CNTs show abundant pores with large surface-to-volume ratios, this in turn enhances the process of adsorption/desorption of gases onto the CNTs surface [73-74]. Such process could change the physical properties of the CNTs surface and paves the way toward applications of CNTs in the field of gas sensors [75-76]. It is stated that, sensor based on CNTs and/or their derivatives are characterized by faster response as compared with traditional sensors. It is stated that, significant variations in the electronic properties of the CNTs is recorded when it acts as gas sensor. Accordingly, DFT calculations based ATK-VNL and Gaussian approach has been used to verify the sensing phenomena of CNTs and used effectively to follow the changes in the electronic properties. A case study is reported for H_2S sensing for pristine and functionalized zigzag [77]. The gas molecules that adsorb on the surface of CNTs, change the shape of CNTs and trigger redistribution of electrons, leading to a macroscopic change in their resistance. Batch experiments was confirmed by DFT calculations in order to conduct quantitative correlation between structural parameters and CNTs adsorption performance [78]. Molecular modelling analyses of the electronic properties of the CNTs leading the research towered further applications of CNTs. Based on high response, selectivity, high surface area it is reported that, CNTs are excellent candidate for different applications in many areas such as environmental monitoring, space, biomedical and pharmaceutical applications [79-88].

DFT is also confirming some experimental findings for the suitability of CNTs in biological applications. In this sense, beside experimental work, a detailed study on the interaction between pyrimethamine anticancer drug and (6, 0) zigzag single-walled carbon nanotube was performed by DFT/B3LYP and DFT/M06-2X with 6-31G* level of theories [89].

7. Graphene based systems

DFT calculations were carried out for both graphene as well as their complexes to study their abilities for adsorptions of some ions. Coronene was used as graphene model system, complexation was described as exothermic and spontaneous in most cases. The spectral analysis indicated significant variation in electronic properties based upon complexation [90]. The first-principles DFT calculations was used to investigate the mechanism of oxygen reduction reaction in fuel cells. For such reason, copper-nitrogen embedded graphene (CuN_3-Gra) is introduced as an efficient electrocatalyst [91]. Molecular modelling analyses dedicate graphene as a catalyst according to its amazing properties including its like large surface area, high thermal and electronic conductivity, high mechanical strength and excellent chemical stability [92]. It is stated that, graphene is almost inert regarding the process of adsorption owing to the in-plane π-conjugation. It is suggested to enhance the surface reactivity of graphene, this is could be conducted as one replacing one or more of carbon atoms with heteroatoms, this could dramatically change the electronic properties [93-94].

As well as other members of carbon nano materials graphene show the potential applications as gas sensor. It has high specific surface area, extremely low Johnson noise, unusual carrier density dependent electrical conductivity and limited crystal defects [95-100]. Molecular modelling data dedicate graphene for novel and unusual applications. It could be applied as a heavy metal detector [101]. While it is reported that such applications could be carried out with graphene quantum dots [102]. Molecular modelling suggested that, the interaction of graphene with heavy metals leads to variation in electronic properties in terms of charge transfer and Schottky barrier height which leads to the change in the current flowing through the barrier.

Regarding the fullerene, CNTs and graphene it is clear that the investigation of electronic properties is important step toward understating the mechanism of interaction of such structures with their surrounding molecules, then it is important to understand the electronic properties for functionality and further applications of carbon nano materials. It is stated that molecular modelling methods specially those based on DFT are effective methods to investigate electronic properties of carbon nano materials [103-106].

8. Modelling other forms of carbon:

Exfoliated graphite (EG) is a promising material for many applications such as flow field plates for fuel cells, EMI shielding, vibration damping and stress and chemical sensing [107-108]. Owing to these wide range of application EG is exposed to molecular modelling to assess its different properties including the mechanical, thermal and electrical properties respectively [109].

Modelling was supporting experimental finding in order to optimize the application of graphite as electrodes with different thicknesses and porosities for high-energy-density Li-Ion batteries [110]. Diamond D5 substructures was subjected to molecular dynamics simulations [111]. The structural stability of such intermediates/fragments appearing in the construction/destruction of D5 net was investigated. The nanotwinned diamond films under nanoindentation was subjected to molecular dynamics simulations [112].

The rational design of carbon fibers with desired properties requires quantitative relationships between some parameters such as microstructure and resulting properties. Molecular modelling with different levels shows potential applications for predicting the microstructure evolution during the processes of carbonization which in turn is effective tools for tailoring the desired carbon fibers [113-114]. It is also reported that, molecular modelling could be also utilized to study the mechanical behavior of carbon fiber-amine functionalized multiwall carbon nanotube/epoxy composites [115].

9. Conclusion and outlook:

Based upon the above considerations carbon nano materials have unique surface, physical as well as chemical properties which leads to amazing applications. Based on molecular modelling it is clear that, hetero atoms could dramatically alter the electronic properties which leads to further applications covering many areas of science and technology. It is stated that some important and simple parameters such as total dipole moment, band gap energy and molecular electrostatic potential could be important to understand the functionality of carbon nano materials [116-118].

It is now well known to utilize quantum mechanical methods for tailoring materials with special functions to act for certain applications. For examples the discovery of two-dimensional (2D) materials such as graphene, silicene, molybdenum disulfide, black phosphorus, and graphitic carbon nitride have received tremendous attention owing to their exceptional features with respect to quantum transport, photoelectric activity, and photocatalysis [119-120]. There are systematic errors within these molecular modelling methods which could be corrected with scale factor. For methods like DFT: B3LYP [121-123] the accuracy is comparable with experimental results after scaling the calculated results. So that, molecular modelling with different levels and routes are now ready to design new materials for future purposes. Finally, this review indicated that molecular modelling is a useful tool for studying carbon based materials as well as their derivatives. It is also of concern for many other systems and structures whereas the experimental tools are limited and/or unavailable [124-130].

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