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The effect of Glutamine on conductivity and energetic properties in Graphene: A DFT studies

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Abstract

Using the Computational methods, the interaction effect of Glutamine Amino acid on Graphene was investigated. For this purpose, the Density Functional Theory) DFT) in the ground state of 6-31G was used, and the interaction effects of Glutamine on Graphene was investigated through attachment to two different base positions. Different parameters such as energy levels, the amount of Chemical Shift in different atoms, the amount of HOMO/LUMO values and related parameters like Electrophilicity scale, chemical hardness, Chemical potential, and the maximum amount of electronic charge transferred. The results of this investigation also show that the attachment of Glutamine Amino acid, as an organic compound, to the chemical structure of Graphene can change these capabilities to a great extent and also increase the role that this mixture already plays in medical, Pharmaceutical, and electronic industries.

Keywords: DFT, Glutamine, HOMO/LUMO, Electrophilicity

1. Introduction

Nanostructures can be categorized into following forms according to their structures: diamonds with sp3 hybridization, Graphites with sp2 hybridization, Hexagonal diamonds with sp3 hybridization, fullerenes with sp2 hybridization, Nanoparticles, Graphenes, single layer and multi-layer nanotubes, Crystal Nanostructures. All these forms of nanostructures produce unique Pharmaceutical and electronic properties. Graphenes have a two-dimensional structure of a single layer of carbon chicken wire [1-5]. The production of Graphene from First Glutamine-functionalized graphene in different positions standard genetic code. It is not recognized as an essential amino acid, but may become conditionally essential in certain situations, including intensive athletic training or certain gastrointestinal disorders. Glutamine is best known for its ability to serve as a source of fuel for the cells that line the gastrointestinal tract. More (carboxyl site equal AGER and NH2 site equal BGER) were simulated and the measurement of calculation related to geometrical optimization, nuclear magnet resonance (NMR) and Natural bond orbitals (NBO) were performed. The Electrophilicity parameter was first defined and investigated by Parr et al. the Electrophilicity parameter can be used in the investigation of the most of the systems and also in the description of the chemical reactions in different organic ways. Besides, in some of the chemical reactions, this factor has been regarded as an effective factor in the amount of outcome in Diels–Alder reactions. The Electrophilicity parameter is caused by the electronic structure of the substance and is independent from the effects of molecular nucleus. In a series of studies, Domingo et al investigated the relation among the electronic effects of substitutions, electrophilicity parameter, and Hammett equation in a mixture of ethylene. The Electrophilicity values, the maximum amount of electronic charge transferred, chemical hardness, and also Chemical potential can be calculated using the relations 1 to 4. In these relations, the (I) represents “ionization potential” and (A) stands for “electron affinity” [13-30].

$$\mu = (\varepsilon H + \varepsilon L)/2 \quad (1)$$

$$\eta = \varepsilon L - \varepsilon H \quad (2)$$

$$\omega = \mu 2/2\eta = \chi 2/2\eta \quad (3)$$

$$\chi = -\mu = -(\delta E/\delta N)V(r) \approx (I+A)/2 \approx -1/2\ (\varepsilon HOMO + \varepsilon LUMO) \quad (4)$$

$$\eta = (\delta 2E/\delta N2)V(r) = (I-A) \approx (\varepsilon LUMO - \varepsilon HOMO) \quad (5)$$

$$\Delta Nmax = -\mu/\eta \quad (6)$$

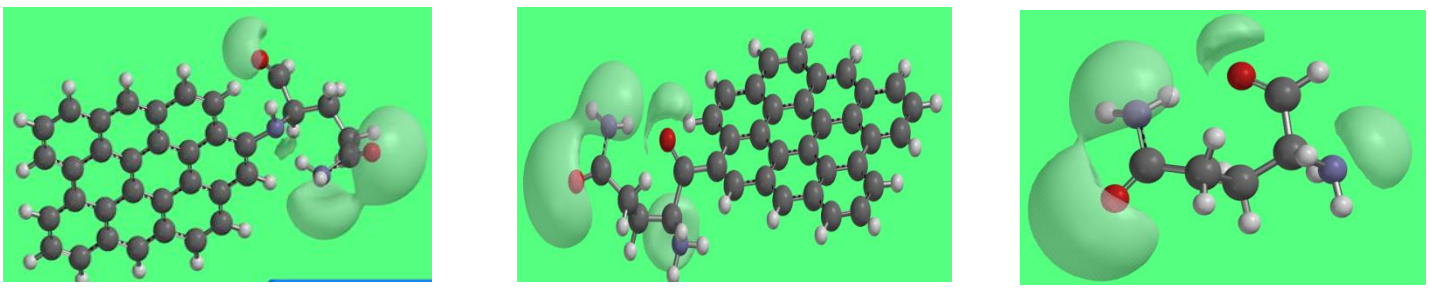

Fig. 2. Potential surfaces in Glutamine, A ger and B ger

Computational details

All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade.. After the initial optimization of the mixtures, the Gaussian 09 software is used for final optimization. For the calculation of HOMO/LUMO values, the Gauss sum software is used [18, 21].

Result and discussion:

The related structures are named in the following way:

One of the parameters that can be calculated by Computational chemistry is the value of HOMO and LUMO and their related parameters such as chemical hardness, Chemical potential, Electrophilicity, the most amount of surrounded electric charge, and the energy gap. The results of the study are tabulated in the table NO 1.

Table 1. Values of energies of the frontier molecular orbitals (εHOMO and εLUMO, eV), electronic chemical potential, μ (eV), chemical hardness, η (eV), electrophilicity, ω (eV) and maximum amount of electronic charge transfer and different position energies for all of Geraphene structures calculated at the B3LYP/6-31G level of theory.

	Glutamine	**B GER**	**A GER**
Dipole moment(deby)	-4.1271	5.624	**3.1781**
S(cal/mol-kelvin)	101.5	179.371	**177.284**
HLG(a.u)	0.1743	0.08794	**0.08629**
EHOMO(a.u)	-0.0417	-0.1645	**-0.1775**
ELUMO(a.u)	-0.2160	-0.0785	**-0.0912**
ΔNmax	-4.3694	2.7859	**3.11403**
Electrophilicity	-0.02948	0.1706	**0.2091**
Chemical potential	-0.12881	-0.1225	**-0.1343**
Chemical hardness	-0.08715	0.04397	**0.04314**

As the figure No 1 shows, the attachment of Glutamine changes the trend of values related to HOMO and LUMO. For comparing the energetic level of structures, after the optimization of the structures by Density Functional Theory at a theory level of B3LYP, different structural forms are compared with one another. The results of this comparison which are tabulated in table 1 show that the attachment of Glutamine structure to the structure of Graphene changes the values of energy.

Fig. 2. Displays the trend of the HOMO/LUMO changes in the various charts.

The results show that the attachment of Glutamine structure to the structure of Graphene reduces the total energy level. The values of Entropy also show that the attachment of Glutamine structure to the structure of B GER increases the amount of disorder and chaos and consequently the value of Entropy. The values of dipole moment also show interesting results. B GER shows greater dipole moment value in comparison to other forms. In other forms, in comparison to form in which Glutamine is not attached to Grapheme, the attachment of Glutamine to Graphene from A GER position does not change the value of dipole moment so much.

1. Conclusion

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Graphene was done separately and only when the structure of Glutamine was attached to it and the results of this computation can be classified as follows:

investigation of all the parameters show that the attachment of Glutamine The structure to Graphene structure will influence the energy levels and dipole moment changes and these changes are able to be investigated in the electrical and chemical parameters of Graphene structure.

The attachment of Glutamine structure is a reason for the changes in the energy levels and also HOMO and LUMO values.

The investigation of energy levels and HOMO/LUMO values show that the attachment of Glutamine structure to Graphene structure form different positions of base will yield different results for chemical hardness, chemical potential, Electrophelicity, and ΔNmax, in accordance to the attachment position; and the most appropriate position is the most symmetrical one.

We expect that the changes in chemical parameters change the physical, electronic, and even pharmaceuticalproperties of Graphene and Glutamine, and these changes are able to be investigated by the specialists of these fields.

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