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Investigation of Adsorption Enthalpy of Prolin on the Surface of Graphene with and without Si: A DFT Study

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Abstract

The project is comparing three types of calculation derived graphene. To evaluate the effect of silicon element to Thermochemistry parameters of absorption of prolin in these derivatives. These derivatives of graphene carbon prolin connection made, the difference is only the position of prolin (named GPC1 , GPC2 , GPC3). But in other Derivations first put silicon instead of carbon position, then is added to the silicon(named GPSi1 , GPSi2 , GPSi3).

Keywords: Prolin, Graphene, Silicon, adsorption enthalpy

1. Introduction

In recent year, Nano structure two-dimensional honeycomb lattice of carbon and consists of a single layer. Due to the extraordinary material properties and electrical conductivity thermal conductivity, high density and irritability charge carriers, optical conductivity and mechanical properties of the material has become unique. For this purpose, in this study, prolin levels once in a hexagonal graphene carbon in the position meta and *para*-connected and then by replacing silicon instead of carbon in graphene in the same position again NO_2 molecules on the surface of silicon meta and *para*-connected in two modes, different scenarios to

optimize the geometry and the calculation of the energy consumption in order to calculate thermochemistry parameters were performed on them. The thermal energy of the cases studied, enthalpy, entropy, Gibbs free energy and thermal energy in the calculation of carbon and silicon case, and were compared. In this study, density functional theory and calculation method of calculating the level B3lyp / 6-31g and in the gas phase is done [1-11].

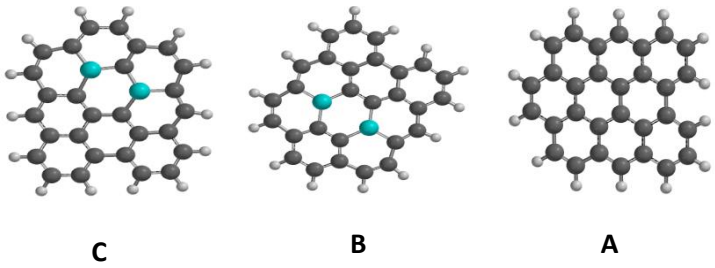

Fig 1. A: Ger B: Ger Si_2 Para C: Ger Si_2 Meta

1.1. Research stage

To make the project easily be checked, four-derived graphene and abbreviations are defined separately.First compound that is formed from prolin is absorbed on the surface of graphene (Ger) (Figure 1). In the *para* position relative to each other, with the latin letter P is displayed second compound which consists of 2 Nitrite is absorbed on the surface of graphene (Ger) (Figure 1). In the *meta* position relative to each other, with the latin letter M is displayed. The third compound that consists of 2 Nitrite is absorbed on the surface of Ger Si_2 P (Figure 1). In the *meta* position relative to each other, with the Latin letter P* is displayed. Fourth compound that consists of 2 Nitrite is absorbed on the surface of Ger Si_2 M (Figure 1). In the meta position relative to each other , with the Latin letter M* is displayed Figure 2.

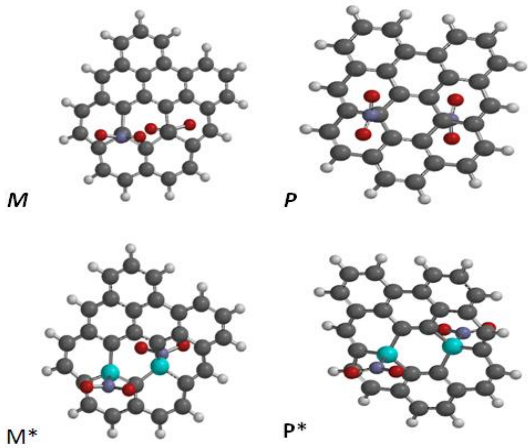

Fig 2. Derivatives investigated in this study P: Ger $(NO_2)_2$ para, M: Ger $(NO_2)_2$ Meta, P*: Ger Si_2 $(NO_2)_2$ Para, M*: Ger Si_2 $(NO_2)_2$ Meta

2. Computational details

In order to study the adsorption enthalpy, the prolin on nano-graphene in 3 positions to put together and optimize computing and energy calculations were performed for those states.Then replacing silicon with graphene carbon in 3 positions calculations before was similar calculations were performed. The results of the calculations are in below. All caculations were performed by using Gaussian 98. using density functional theory and 6-31g in gas phase temperature 298 K and pressure 1 atm.

3. Results and discussion

3.1 Calculation and values enthalpy changes (ΔH)

Using Gaussian 98 program enthalpy values for graphene, prolin and any of the compounds were calculated. The first results of enthalpy: To calculate and obtain the enthalpy change in the reaction A + B → AB of the following formula is used:

$\Delta HAB = [HAB] - [HA + HB]$

Given the reaction Ger+ pro→ GPC+ H_2 values of enthalpy obtained through calculation software Gaussian, for example, to combine GPC, we have:

ΔHGPC= [H GPC+ HH2] – [HGer +Hpro]
Δ HGPC1= [(-1475.39 a.u)+ (-1.10 a.u)]– [(-1151.14 a.u)+ (-400.87 a.u)]= 75.52 a.u
Δ HGPC2= [(-1476.13 a.u)+ (-1.10 a.u)]– [(-1151.14 a.u)+ (-400.87 a.u)]= 75.78 a.u
Δ HGPC3= [(-1476.13 a.u)+ (-1.10 a.u)]– [(-1151.14 a.u)+ (-400.87 a.u)]= 75.78 a.u

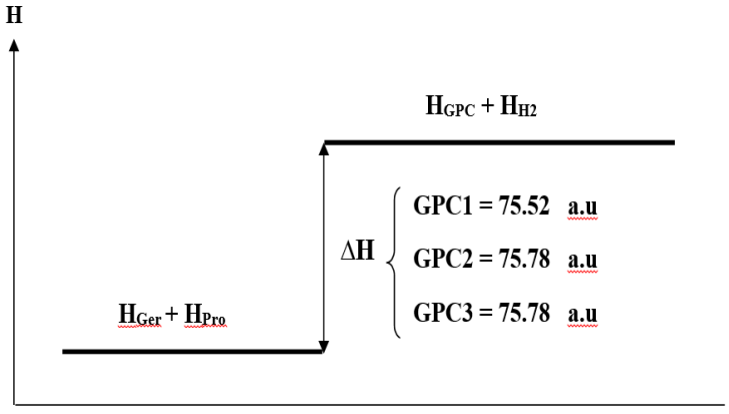

Fig.3. Diagrams the enthalpy change for a combination of P.

ΔHGPC value indicates that the process of adsorption of prolin for graphene in the para position relative to each other is endothermic. According to ΔH values obtained and compare them together, it is clear that

carbon adsorption on graphene prolin, in the meta and para position, the enthalpy changes with the same situation.

3.2. The second results of enthalpy

According to the above equations according to reaction Ger Si+ pro→ GPSi and enthalpy values obtained through calculation software Gaussian, for the combination of GPSi, we have:

As a result of the placement of the numbers we have:

Δ HGPSi = [HGPSi + HH2] – [HGer + Hpro]
ΔHGPSi1 = [(-1726.74 a.u) + (-1.10 a.u)] – [(-1402.46 a.u) + (-400.87 a.u)] =77.69 a.u
ΔHGPSi2 = [(-1727.50 a.u) + (-1.10 a.u)] – [(-1402.45 a.u) + (-400.87 a.u)] =76.92 a.u
ΔHGPSi3 = [(-1727.48 a.u) + (-1.10 a.u)] – [(-1402.37 a.u) + (-400.87 a.u)] =76.86 a.u

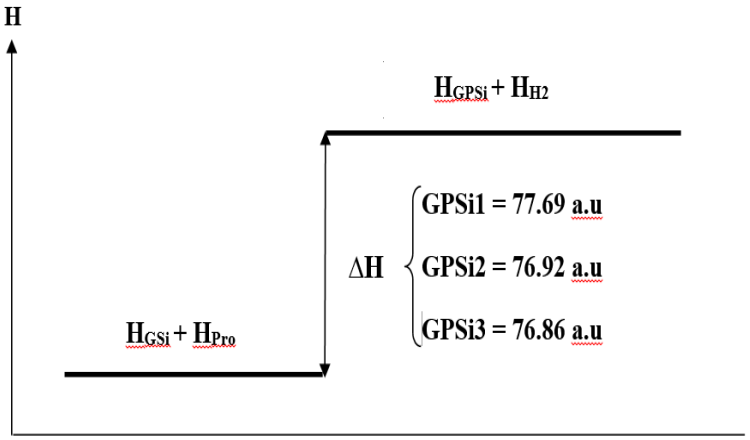

Fig.5. Diagrams the enthalpy change for a combination of GPSi

The ΔHGPSi indicates that the process of adsorption on graphene Si with prolin relative to the endothermic process. The third results of enthalpy: In this category if the combination of GPC and GPSi in terms of ΔH values obtained in the above comparison, we conclude that the combination of compound GPC , GPSi has much less power, so we have:

$\Delta H_{GPSi} > \Delta H_{GPC}$

Δ HGPC1= 75.52 a.u
Δ HGPC2= 75.78 a.u
Δ HGPC3= 75.78 a.u
ΔHGPSi1= 77.69 a.u
ΔHGPSi2= 76.92 a.u

ΔHGPSi3= 76.86 a.u

Chart and table below for the four combined values of ΔH P, M, P * and M * shows.

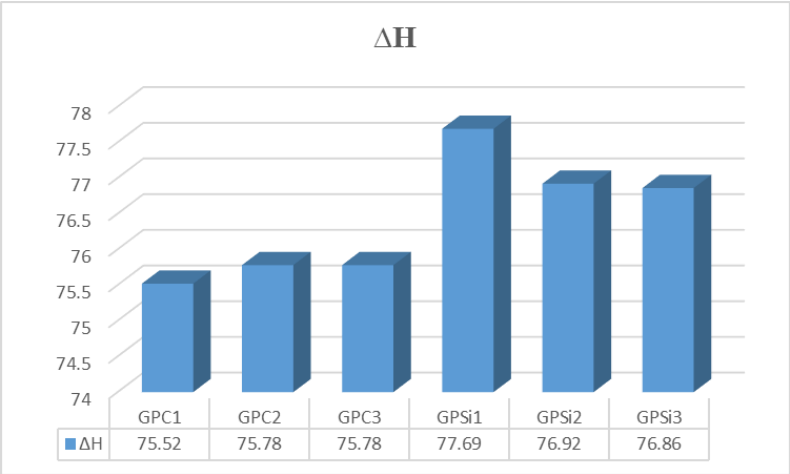

Table 1. Compounds ΔH values GPC1,GPC2,GPC3,GPSi1,GPSi2,GPSi3 according a.u

Enthalpy changes: ΔHGPSi> Δ HGPC

4. Conclusion

Compare enthalpy values for different scenarios studied indicate that GPSi has more ΔH than GPC. So prolin better absorbed when the composite graphene has silicon.

Acknowledgment

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