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Theoretical study of the effect of the element silicon, the adsorption enthalpy nitrite, on the surface of graphene nanostructure

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Abstract

The project is comparing four types of calculation derived graphene. To evaluate the effect of silicon element to Thermochemistry parameters of absorption of nitrite in these derivatives. Two of these derivatives of graphene carbon nitrite connection made, the difference is only in the state of Para and meta carbons connectivity state (named P & M). But in other Derivations first put silicon instead carbon in the meta and para position(named GER Si_2 para & GER Si_2 metha), then nitrite is added to the silicon(named P & M*).*

Keywords: ***nitrite***, graphene, silicon, adsorption enthalpy

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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, nitrite NO2 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 NO2 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].

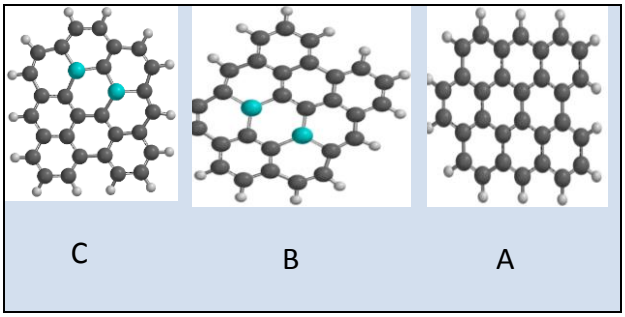

Figure 1. A: Ger B: Ger Si2 Para C: Ger Si2 Meta

2 Research stage

To make the project easily be checked, four-derived graphene and abbreviations are defined separately.

A) First compound that is formed from 2 Nitrite 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
B) 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.
C) 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.
D) 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.

3 Results:

In order to study the adsorption enthalpy, the nitrite ion on graphene nanostructure in two positions meta and para to put together and optimize computing and energy calculations were performed for those states.Then replacing silicon with graphene carbon meta and para positions calculations before Was Similar calculations were performed. The results of the results of the calculations are in below.

All calculations were performed by using Gaussian 98. using density functional theory and 6-31g in gas phase temperature 298 K and pressure 1 atm.

3.1 Calculation and Values enthalpy changes (ΔH):

Using Gaussian 98 program enthalpy values for graphene, nitrite and any of the compounds were calculated.

3.2 The first results of enthalpy:

To calculate and obtain the enthalpy change in the reaction A + B →AB of the following formula is used:

$\Delta H_{AB} = [H_{AB}] - [H_A + H_B]$

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Given the reaction Ger + $2NO_2 \rightarrow$ Ger $(NO_2)_2$ values of enthalpy obtained through calculation software Gaussian, for example, to combine P, we have:

ΔH_P = [H Ger(NO2)2 Para] – [H_{Ger} +2 H_{NO2}]

ΔH_P = [1157.10782 kJ/mol] – [(1070.153887 kJ/mol) +2(26.73809404 kJ/mol)] =33.4593745 kJ/mol

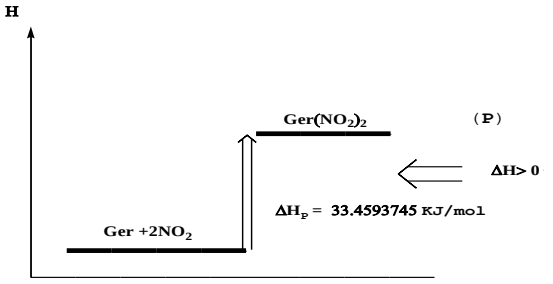

Figure 3. diagrams the enthalpy change for a combination of P

ΔHp value indicates that the process of adsorption of nitrite for graphene in the para position relative to each other is endothermic. also were combined in Meta positions M:

ΔH_M = [1157.10782 kJ/mol] – [(1070.153887 kJ/mol) +2(26.73809404 kJ/mol)] = 33.4593745 kJ/mol

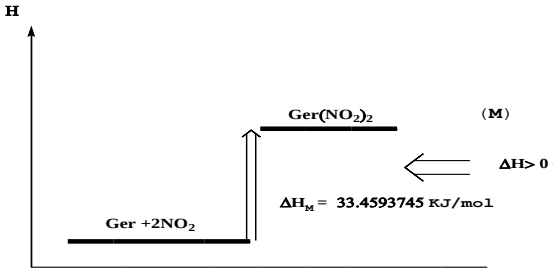

Figure 4. diagrams the enthalpy change for a combination of M

ΔH_M value indicates that the process of adsorption of nitrite for graphene in the meta position relative to each other is endothermic. According to ΔH values obtained and compare them together, it is clear that carbon adsorption on graphene nitrite, in the Meta and para position, the enthalpy changes with the same situation.

3.3 The second results of enthalpy:

According to the above equations according to reaction Ger Si_2 + $2NO_2$ → Ger Si_2 $(NO_2)_2$ Meta and enthalpy values obtained through calculation software Gaussian, for the combination of M *, we have:

ΔH_{M^*} = [H GerSi2 (NO2)2 Meta] – [$H_{Ger\,Si2}$ +2 H_{NO2}]

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

ΔH_M = [H Ger (NO2)2 Meta] – [H_{Ger} +2 H_{NO2}]

ΔHM*= [1119.42927 kJ/mol] – [(1034.92492 kJ/mol) +2(26.73809404 kJ/mol)]= 31.0281614 kJ/mol

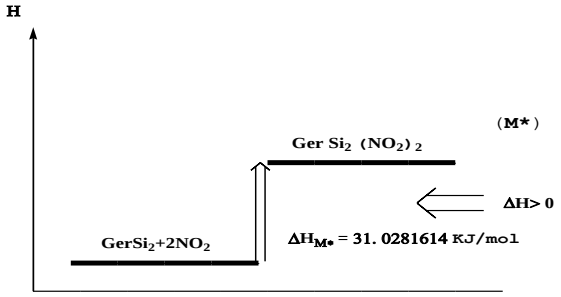

Figure 5. diagrams the enthalpy change for a combination of M*

The ΔH_{M^*} indicates that the process of adsorption on graphene Si with two nitrite in the meta position relative to the endothermic process. also were combined in para positions P*:

ΔHP*= [H Ger Si2 (NO2)2] – [H Ger Si2 +2 H_{NO2}]

ΔH_{P^*} = [1127.10623 kJ/mol] – [(1034.84615 kJ/mol) +2 (26.73809404 kJ/mol)] = 38.783889 kJ/mol

The ΔH_{P^*} indicates that the process of adsorption on graphene, Si with two nitrite in the para position relative to the endothermic process. And also due to ΔH values and comparing them together, it is clear that the nitrite doped graphene on silicon alternatives on the screen in

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two positions meta and para, the enthalpy changes with different status.

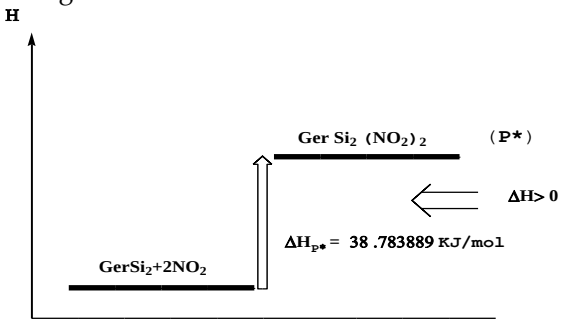


Figure 6. diagrams the enthalpy change for a combination of P*

3.4 The third results of enthalpy:

In this category if the combination of P and P * in terms of ΔH values obtained in the above comparison, we conclude that the combination of compound P, P * has much less power, so we have:

$\Delta H_P = 33.4593745$ kJ/mol

$\Delta H_{P^*} = 38.783889$ kJ/mol

$\Delta H_{P^*} > \Delta H_P$

3.5 The fourth results of enthalpy:

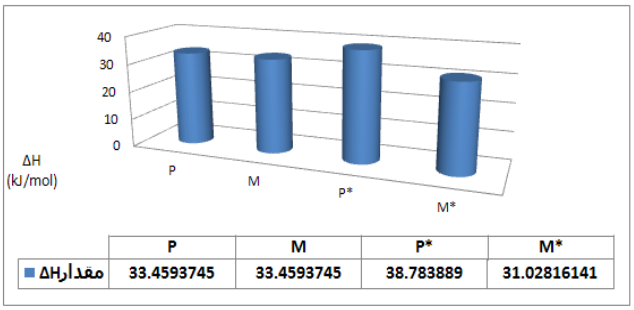
In this category if the combination of M and M * in terms of ΔH values obtained in the above comparison, we conclude that the combination of compound M *, M has much less power, so we have:

$\Delta H_M = 33.4593745$ kJ/mol

$\Delta H_{M^*} = 31.0281614$ kJ/mol

$\Delta H_M > \Delta H_{M^*}$

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



$\Delta H_{P^*} > \Delta H_P = \Delta H_M > \Delta H_{M^*}$: Enthalpy changes

Figure 7. Final Compare the amount of enthalpy in compounds of interest in this article

4 Conclusion:

Compare enthalpy values for different scenarios studied indicate that the mode M * more likely, the state P, M possible to achieve the same P * is more difficult than other states. so when the composite graphene with silicon adsorption at interfaces meta Creating better absorbed shows.

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