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Original Research Article

A Thermodynamic Study on Nano-graphene Interaction with the Amino acid Phenylalanine in Acidic and Alkaline conditions at different temperatures

Mahnaz Sadat Zolfaghari*

Department of chemistry, Faculty of chemistry and petroleum sciences, Shahid Beheshti university, General campus evin, Tehran, Iran

*Corresponding author Fax number: Tel.: +98 937 965 9317

*E-mail: Mahnazzolfaghari627@yahoo.com

ABSTRACT

The project is comparing two types of calculation derived graphene. Which one of these carbon graphene linked to the phenylalanine amino acid from the acidic site (-COOH) and another from the base site ($-NH_2$). For this purpose, at first the material contained in the both sides of reaction were geometrically optimized, then the calculation of the thermodynamic parameters performed on all of them. The amount of ΔH, ΔS and ΔG of this reaction at different temperatures in form of sum of parameters discrepancy in the products than reactants are obtained, and finally, the best temperature for the synthesis of derivations of phenylalanine - Graphene according to the obtained thermodynamic parameters were evaluated.

Keywords: phenylalanine amino acid, Graphene, base & acid binding position, density functional theory.