CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME IV

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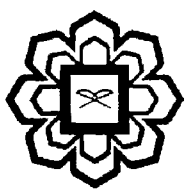

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CHAPTER 17

COMPUTATIONAL STUDIES OF ADSORPTION GLYCINE ON CARBON NANOTUBES

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ABSTRACT

Functionalized carbon nanotubes (CNT) hold strong promise as novel systems for the delivery of drugs, antigens and genes. In this work, quantum chemical methods were applied to study the interaction between Glycine (N-centered and C-centered) with CNT(4,4). Glycine radicals were directly added to CNT surface and the results show N-centered glycine radical is preferably gets attached to CNT and found to be more stable compared to C-centered glycine. Additionally, CNT(3,3) has been functionalized by attaching nonionic and zwitterionic form of glycine on top of its surface. The zwitterionic form of glycine is more negative at the oxygen end and thus more stable compared to glycine in nonionic form. The binding energies and geometrical parameters obtained in this project are in excellent agreement with previous experimental and theoretical studies.

Keywords: binding energy, CNT, functionalization, glycine, modelling

INTRODUCTION

Functionalization of CNTs is a way to overcome difficulties which occur when dealing with CNTs such as difficult to disperse and dissolve in water or in organic solvent and also high resistance in wetting. CNT with different surface modification can be used for different field. Many studies have been done to model the adsorption properties of amino acid on CNT structures. For instance, the effects of the adsorption of glycine, histidine, phenylalanine, and cysteine on the electronic structure of the metallic CNT(3,3) using density functional theory has been studied by Roman (2006). A density functional study on the interaction of glycine with carbon nanotubes (Mavrandonakis, 2006) found that the C-centered radical is favored over the N-centered one by 22.7 kcal/mol employing the BLYP functional. Upon reaction with the tube walls, the glycine radical forms stable complexes when it reacts with the nitrogen atom and meta-stable conformations with α-C-atom. The C- and N-centered glycine radicals with the (4,4) and (8,0) CNTs, are found to have similar stability.

In this chapter we present the result of the computational studies of the adsorption of glycine radical on CNT and adsorption of nonionic and zwitter ionic forms of glycine on CNT, using semi-empirical quantum chemical methods.