QUANTUM MECHANICAL STUDY OF DIFFERENT TYPES OF PROTEIN SENSORS

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ABSTRACT

Proteins are polymers of amino acids connected by dipeptide bonds. Amino acids play central roles both as building blocks of proteins and as intermediates in metabolism. They are essential for the structure, function, and regulation of the body's tissues and organs. Proteins are made up of hundreds of smaller units called amino acids that are attached to one another by peptide bonds, forming a long chain. There are 20 common amino acids found in proteins, and depending on their sequencing, and the overall protein structure, they convey an extensive array of chemical properties.

Graphene is the youngest known allotrope of carbon which is a two-dimensional and one-thick materials consisting sp^2 hybridized carbon atoms arranged in honeycomb structure. These honeycomb structure are the reasons for the extraordinary properties of graphene, which include a very large surface area [2630m^2/g, it is double that of single-walled carbon nanotube (SWCNT)], a tunable band gap, room temperature Hall effect, high mechanical strength (200 times greater than steel), high elasticity and high thermal conductivity. The exceptional electrical properties of graphene (such as, high charge mobility and capacity, highly tunable conductance) endow it as an ideal sensing element in electronic sensors. Carbon nanostructures [CNSs] exhibit non-covalent interaction such as the XH-π, cation-π, anion-π and π-π interaction towards the small gas molecules, metal ions and bio molecules. The XH-π weak interactions were extensively studied in recent years. These interactions are considered as a unique type of hydrogen bonding interaction in which π electron acts as the proton acceptor. Graphene is a sensitive nano material which detects all the individual events when a biomolecule is adsorbed to or deadsorbed from its surface. The adsorption of various substrates such as amino acids, nucleic acids, antibodies, gas molecules, metal

ions, polymers, organic molecules etc. on grapheme/CNT surfaces has attracted considerable attention because of the fundamental importance and potential industrial applications. In particular, the protein and graphene/CNT interaction has gained significant attention because of its application in various fields such as DNA sequencing, DNA sensing, amino acids sensing, drug delivery etc. Recently, it has been found that the determination of a patient's DNA sequence can reveal one's risk of falling ill with a particular disease and also help to design "personalized medicine", and thus the DNA sequencing appears to be one of most potential applications. The density functional theory (DFT) B3LYP with basis 6-31G** reproduced the proper geometry of the molecules under study. M062X method also provides other properties with accuracy. The charge, geometrical parameters etc. thus obtained can be used for further calculations and interpretations of molecular properties. It has been observed that the interaction energy, adsorption and chemical reactivity varies significantly for alkaline earth metal ions and amino acids with CNTs and graphene. It is expected that the current study will help in development of carbon material based biosensors.