Panvika Pannopard 2007: Structure and Electronic Properties of "DNA-Gold-Nanotube" Systems: A Quantum Chemical Analysis. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Tanin Nanok, Ph.D.
83 pages.

The development of a novel DNA sensor is a crucial issue in the diagnosis of pathogenic and genetic diseases. We used the Density Functional Theory (DFT) to investigate the DNA sensor performance of hybrid structures of a gold atom (Au) deposited on two types of single-walled carbon nanotubes: armchair SWCNT(8,0)/Au and zigzag SWCNT(5,5)/Au and compared these with bare Au. The adenine:thymine (A:T) complex is used to represent the base pair in the DNA double helix. The recognition probe is defined as SWCNT/Au/A in which an adenine molecule is immobilized on the SWCNT/Au supporter via its active N7 anchor point. After thymine hybridization (SWCNT/Au/A:T), the overall modulations are analyzed by comparing them with original systems. The hybrid systems, "SWNCTs/Au", exhibit good stability and sensitivity. This is originated from the co-function of a gold atom, which acts as a powerful electron withdrawing group, and SWNCTs, which act as electron collecting centers. With Mulliken population analysis, it was found that the "SWCNTs/Au" could accumulate the electron density better than the bare gold atom by, at most, four times when forming with the A:T complex. We also applied SWCNTs/Au complex as a sensing material for nucleic acids. The SWCNT/Au structure was more reactive to adenine capturing than the bare Au atom. Especially, the SWCNT(8,0)/Au/A system can accelerate target adenine electrons to the SWCNT(8,0)/Au sensing part. Another gold size which also be attached on both SWCNTs was a triangular gold cluster (Au_3). There are several binding characteristics between them, though the best stable complex of each SWCNT is SWCNT(8,0)/Au_3(ApU) (40.2 kcal/mol) and SWCNT(5,5)/Au_3(ApD) (29.9 kcal/mol). The monitoring of molecular charge modulations after the SWCNT/Au_3/A probe binds with the target thymine molecule infers that the sensing quality of SWCNT(8,0)/Au_3(ApU) and SWCNT(5,5)/Au_3(ApD) is better than the bare Au_3 cluster. The SWCNT(8,0) is more suitable to use as the SWCNT/Au_3 supporter than the SWCNT(5,5) due to its great affinity to Au_3 cluster. The overall results of "SWNCTs/Au" and "SWNCTs/Au_3" lead to the propose that the "SWCNTs/gold" systems could be the potential candidate for a nanostructure-based DNA sensor.

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