THESIS

STRUCTURE AND ELECTRONIC PROPERTIES OF "DNA-GOLD-NANOTUBE" SYSTEMS: A QUANTUM CHEMICAL ANALYSIS

PANVIKA PANNOPARD

A Thesis Submitted in Partial Fulfillment of

the Requirements for the Degree of

Master of Science (Chemistry)

Graduate School, Kasetsart University

2007

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.

_____ _____ ___/ ___/ ___

Student's signature Thesis Advisor's signature

ACKNOWLEDGEMENTS

First, I thank my advisor, Dr. Tanin Nanok, for his continuous support in the graduate program. He was always there to listen to me and to give advice. A special thank you goes to my co-advisor, Prof. Dr. Jumras Limtrakul, who showed me different ways to approach a research problem and the need to be persistent to accomplish any goal. He taught me how to ask questions, express my ideas and especially how to write academic papers. I also thank my other my co-supervisor, Dr. Pensri Bunswansong, who gave insightful comments and reviewed my work. I would like to thank the rest of my thesis committee, Asst. Prof. Dr. Surasak Chiangga who is the representative of the Graduate School of Kasetsart University, for his helpful comments and suggestions. I am also greatly indebted to many teachers in Kasetsart University, Assoc. Prof. Dr. Supa Hannongbua, Dr. Chak Sangma and Asst. Prof. Piboon Pantu.

Besides my project leaders, Dr. Pipat Kongpracha who was most responsible for helping me completes this project. He taught me everything which I should know, made me a better scientist, had confidence in me when I doubted myself, and brought out the good ideas in me. He was always there to meet and talk about my ideas, to proofread and mark up my papers and chapters, and to ask me good questions to help me think through my problems. Without his encouragement and constant guidance I could not have finished this dissertation. I am also grateful for the participation of many members of the Laboratory for Computational and Applied Chemistry (LCAC), Kasetsart University especially Dr. Somkiat Nokbin, Dr. Jakkapan Sirijaraensre and all my best friends, for their encouragement.

During the course of this work at Kasetsart University, I was supported by Kasetsart University Research and Development Institute (KURDI), and the Ministry of University Affairs under the Science and Technology Higher Education Development Project (Petroleum and Petrochemical Consortium funded by MUA-ADB). Additionally, supports by grants from the Thailand Research Fund (TRF Senior Research Scholar to JL) and the National Nanotechnology Center under the National Science and Technology Development Agency are acknowledged. Thanks are also to the Laboratory for Computational and Applied Chemistry (LCAC) and Pirun Cluster, Kasetsart University for offering such good computational knowledge-based systems.

Last, but not least, I thank my family for giving me life in the first place, for educating me, for their unconditional support and encouragement to pursue my interests and for believing in me.

Panvika Pannopard

April, 2007