

FIRST PRINCIPLES STUDIES OF INTERACTION BETWEEN DNA AND CARBON NANOTUBES FOR THE POTENTIAL DNA SENSOR APPLICATIONS

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Recently biosensor applications of carbon nanotube (CNT) devices have been intensively investigated. Since the ultra-sensitivity of CNT field effect transistor (FET) sensor is expected, CNT FET sensor is suggested as a DNA sensor to detect even single nucleotide polymorphism

Here we report the first principles studies to understand the interaction between DNA and CNTs for the DNA sensor applications. Firstly, we have carried out first principles electronic structure calculations on the interaction of individual DNA nucleobases (especially guanine and cytosine) with single walled carbon nanotubes (SWNTs). The binding energies of various configurations including π -stacking and direct bonding ones are compared. Secondly, we have calculated the interaction of the thiolated nucleotides with gold nanoparticles to simulate the DNA sensor applications. From the calculated results of above two systems, we tried to propose the mechanism of binding of single-stranded DNA (ss-DNA) on the SWNTs and the hybridization of complementary DNA on the pre-bound ss-DNA.