CHAPTER 5

CONCLUSION

The DFT/B3LYP-optimized structures of closed-end armchair (3,3), (4,4) and (5,5) SWCNTs and their platinum-clusters (Pt_n, n=1 to 4) decorated structures were obtained and their binding energies are reported. The binding abilities of single platinum atom to SWCNTs based on the most favorable configurations are in order: (3,3) SWCNT > (4,4) SWCNT > (5,5) SWCNT. The polynomial equation fitted for plot of their binding energies (kcal/mol) and their diameters (nm) of $\Delta E_{binding}$= $-159.6+350.602d-212.32d^2$ was obtained.

Adsorption energies for hydrogen adsorbed to platinum atom on Pt_n-decorated (3,3), (4,4) and (5,5) SWCNTs were obtained and reported. As hydrogen molecule likely adsorbed to platinum atom on Pt_4-decorated (3,3), (4,4) and (5,5) SWCNTs were identified, the ZPE energetic, thermodynamic properties and equilibrium constants for hydrogen adsorptions on them were determined and reported. All hydrogen adsorptions are exothermic reaction at 298 K. Only hydrogen adsorptions on the Pt_4/(3,3)SWCNT (ΔG_{298}=-20.47 kcal/mol) and Pt_4/(5,5)SWCNT (ΔG_{298}=-10.03 kcal/mol) are spontaneous processes. Equilibrium constant of hydrogen adsorption on the Pt_4/(3,3)SWCNT ($K_{298}=1.02\times10^{15}$) is very large and 4.51×10^7 times larger than on the Pt_4/(5,5)SWCNT ($K_{298}=2.26\times10^7$). The hydrogen storage on platinum atom of Pt_4 decorated closed-end (3,3)SWCNTs can be expected.

All adsorption of CO, NO_2, O_2, NH_3, N_2, SO_2, N_2O and H_2O adsorbed on platinum atom of Pt_n-decorated (3,3), (4,4) and (5,5)SWCNTs are strong except for CO_2.

Pt_4/SWCNT is the most stable structure for H_2 adsorption on the (3,3)SWCNT, while Os_4/SWCNT is the most stable structure for H_2 adsorption on (4,4) and (5,5)SWCNTs.