Density Functional Study of Functionalization of Carbon Nanotubes with Carbenes

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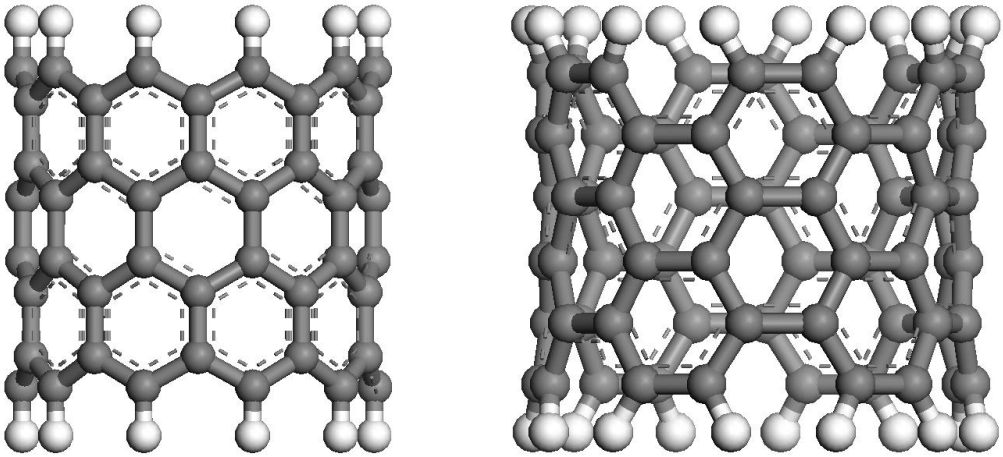
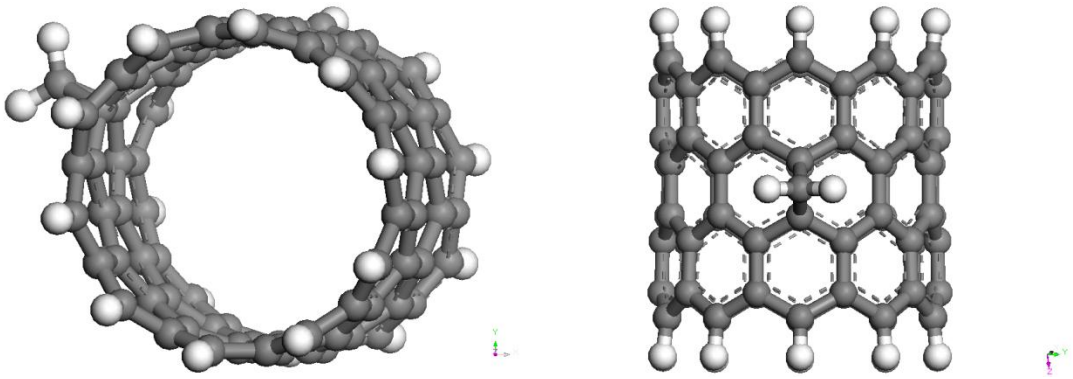


Figure S1 Optimized structures for different models used in this investigation (a)(10,0) CNT and(b) (6,6) CNT



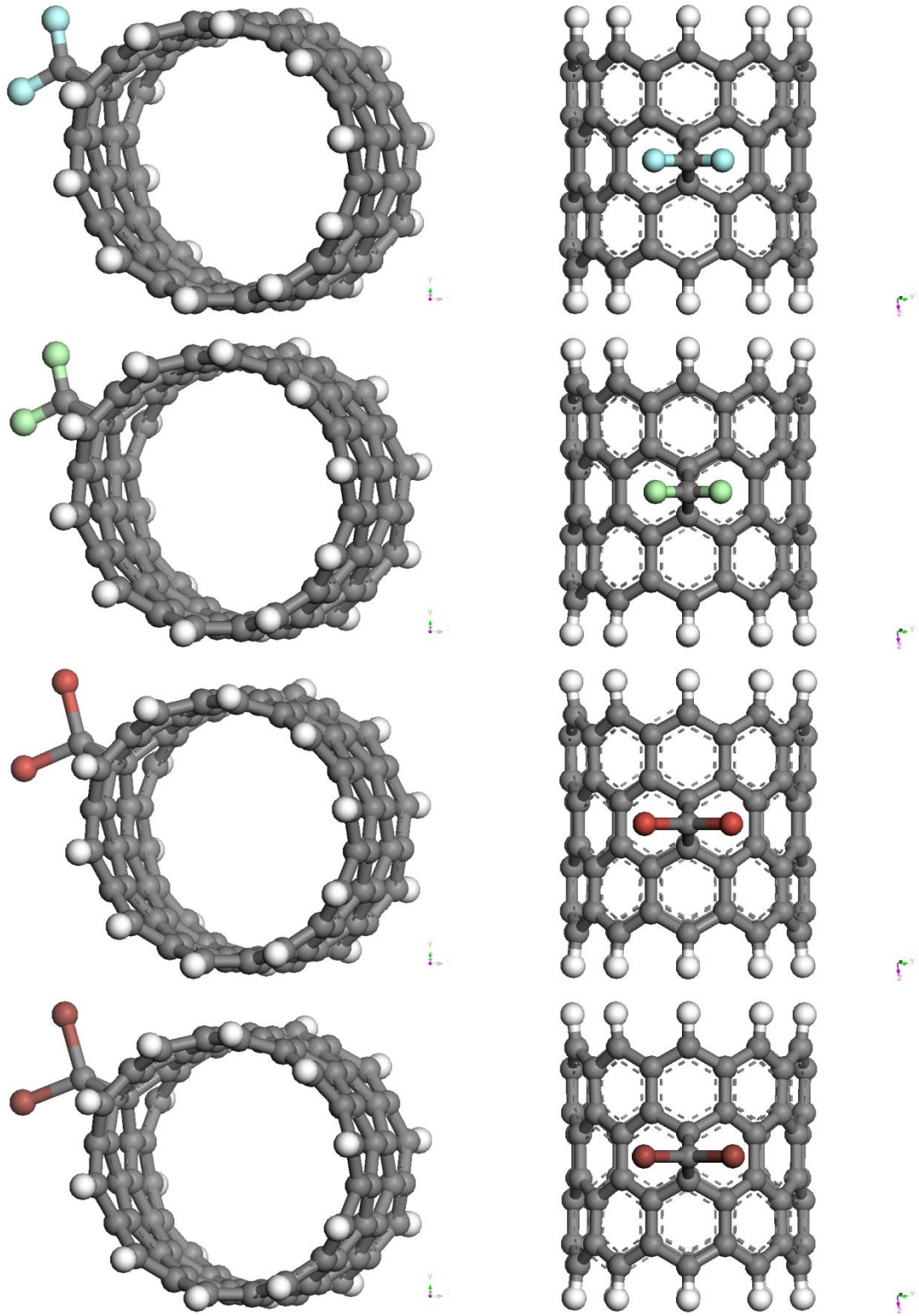


Figure S2 Two views of the products of the functionalization of (10,0) CNT with :CX_2 (from top to bottom- X=H, F. Cl, Br, I)

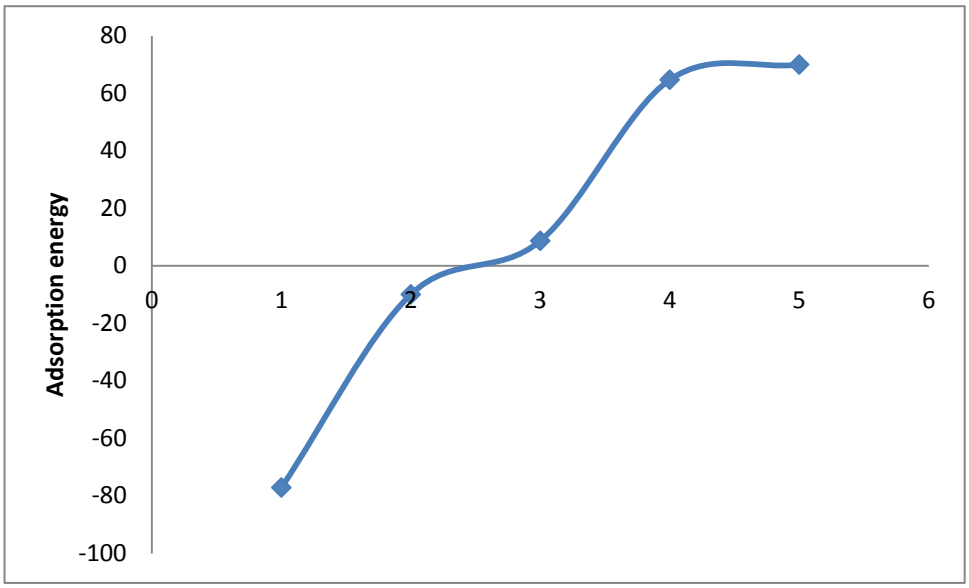


Figure S3 The adsorption energy curve of (10,0) :CX_2 functionalized SWCNT (1- X=H, 2- X=F, 3- X=Cl, 4- X=Br, 5- X=I)

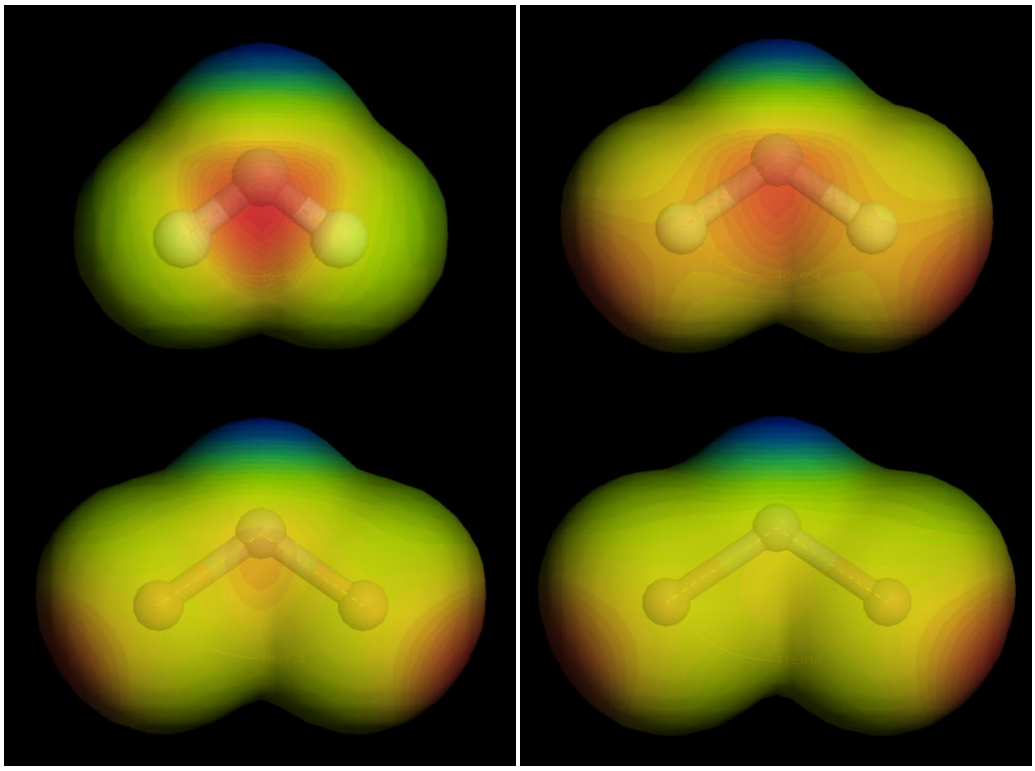


Figure S4 Electrostatic potential maps for the four carbenes (left to right, top to bottom:, :CF_2, :CCl_2, :CBr_2, :CI_2)

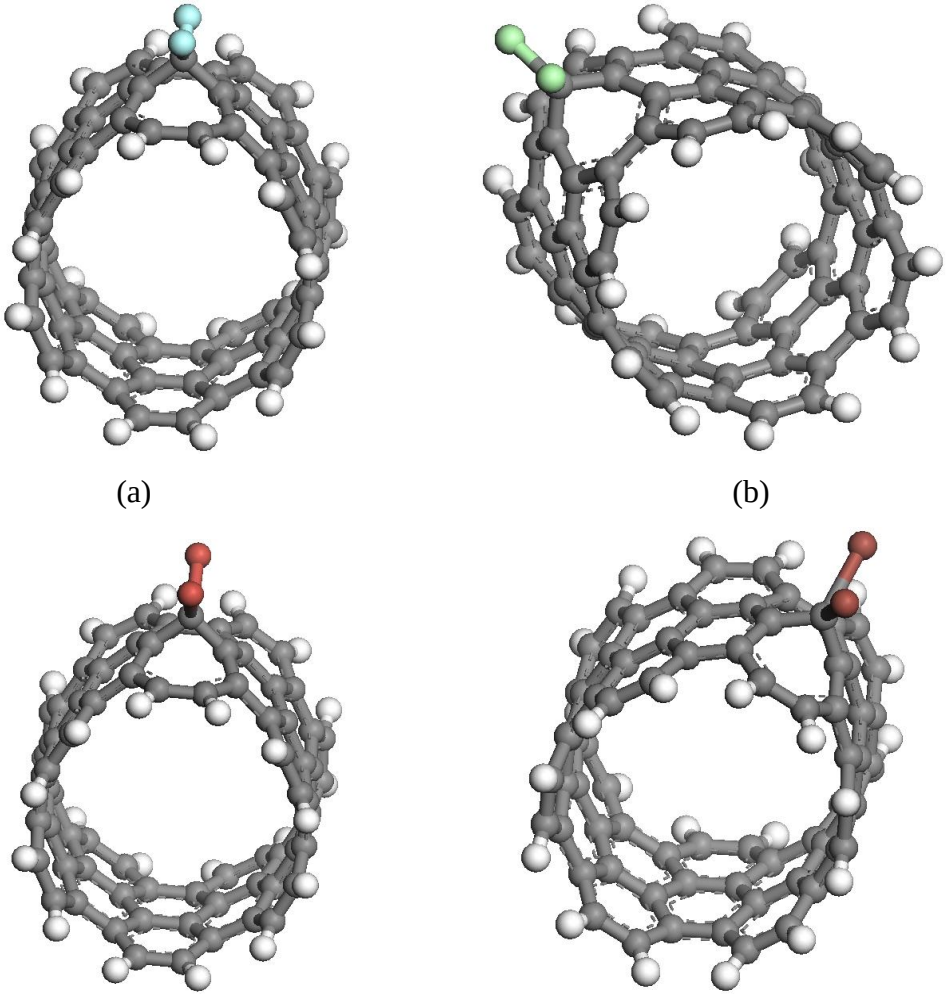


Figure S5 The adsorbed structures on the (6,6) functionalized SWCNT: (a) :CF_2, (b) :CCl_2, (c) :CBr_2, (d) :CI_2

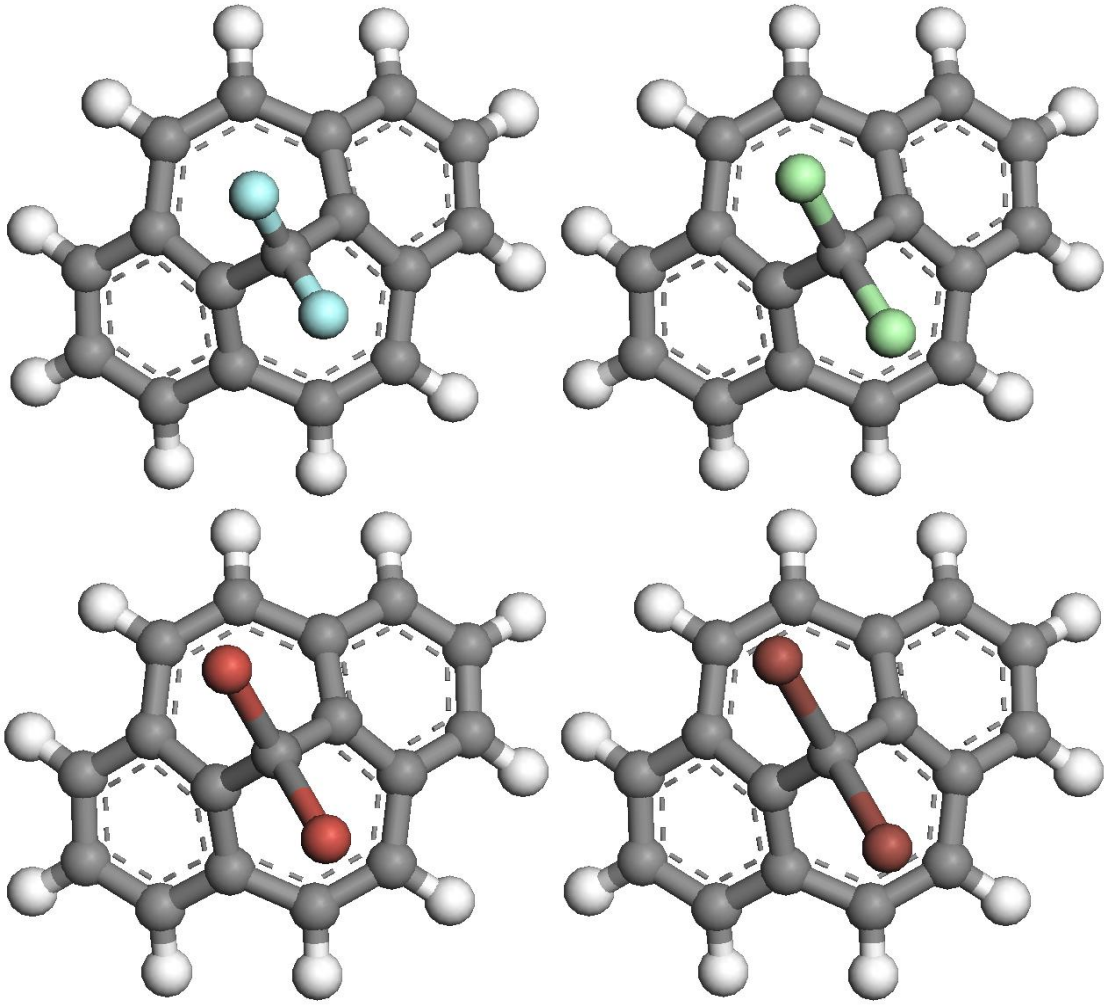


Figure S6 Carbenes, :CX_2 (X = F, Cl, Br, I) adsorbed on the unsaturated analogue

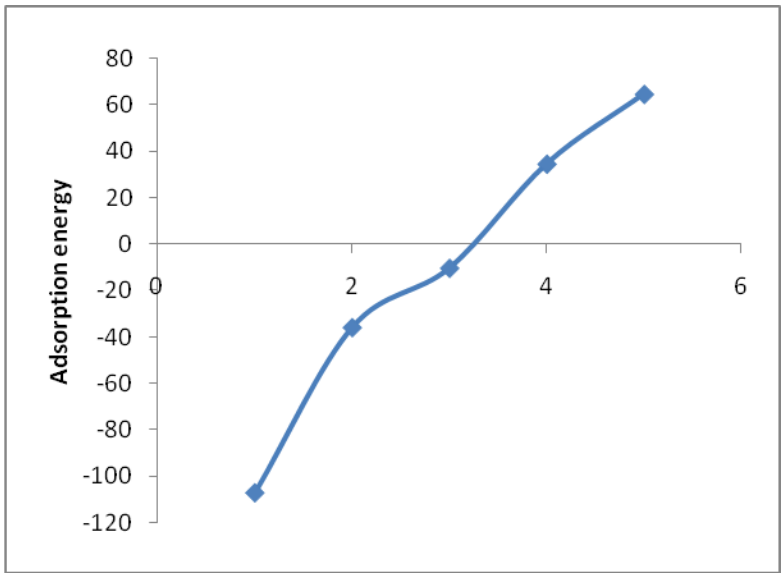


Figure S7 The adsorption energy curve of (6,6) functionalized SWCNT

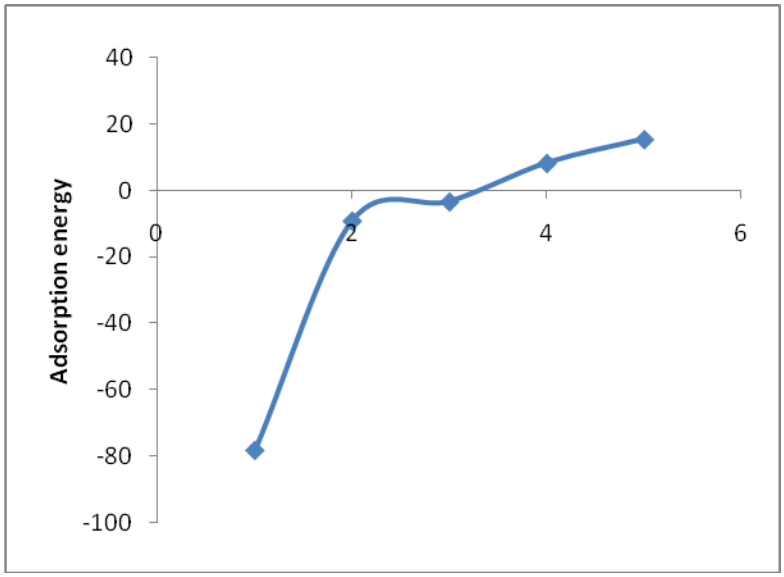


Figure S8 The adsorption energy curve of carbenes adsorbed on $C_{16}H_{10}$

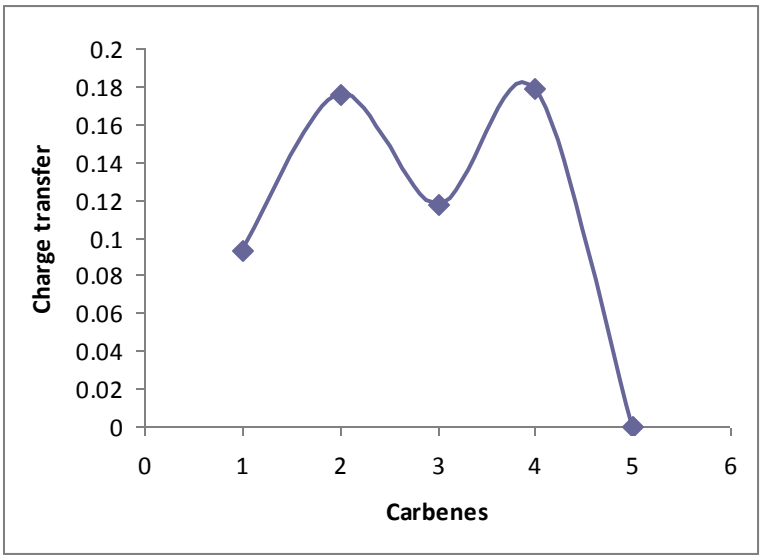


Figure S9 Graphical variation of charge transfer from (10,0) CNT by carbenes

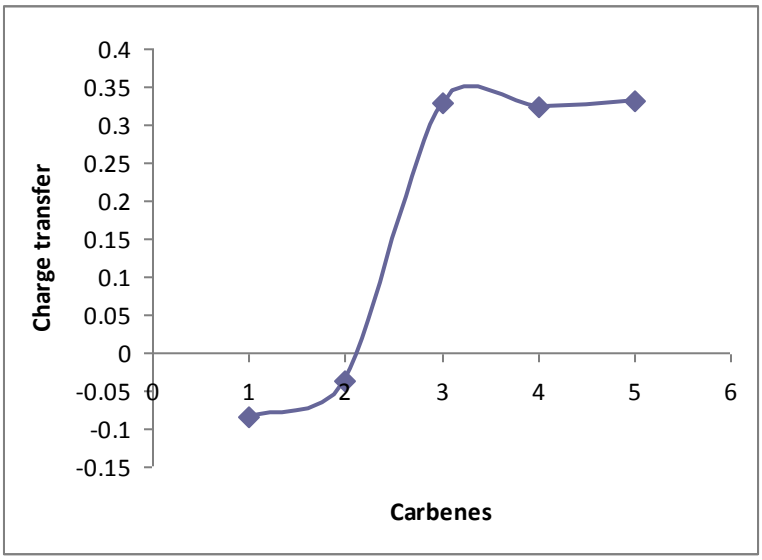


Figure S10 Graphical variation of charge transfer on (6,6) CNT by carbenes

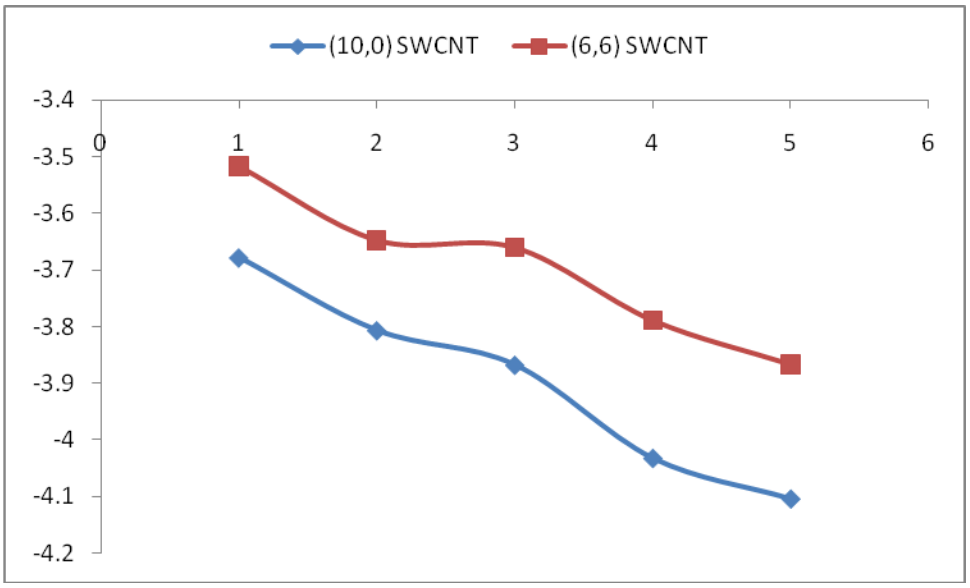


Figure S11 Comparison of the Fermi energies of the (10,0) and (6,6) SWCNTs

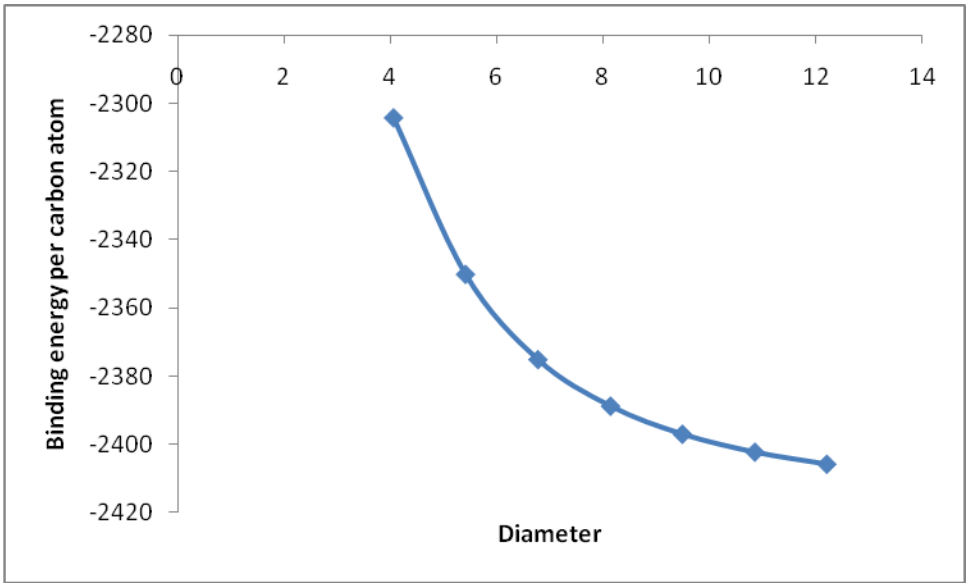
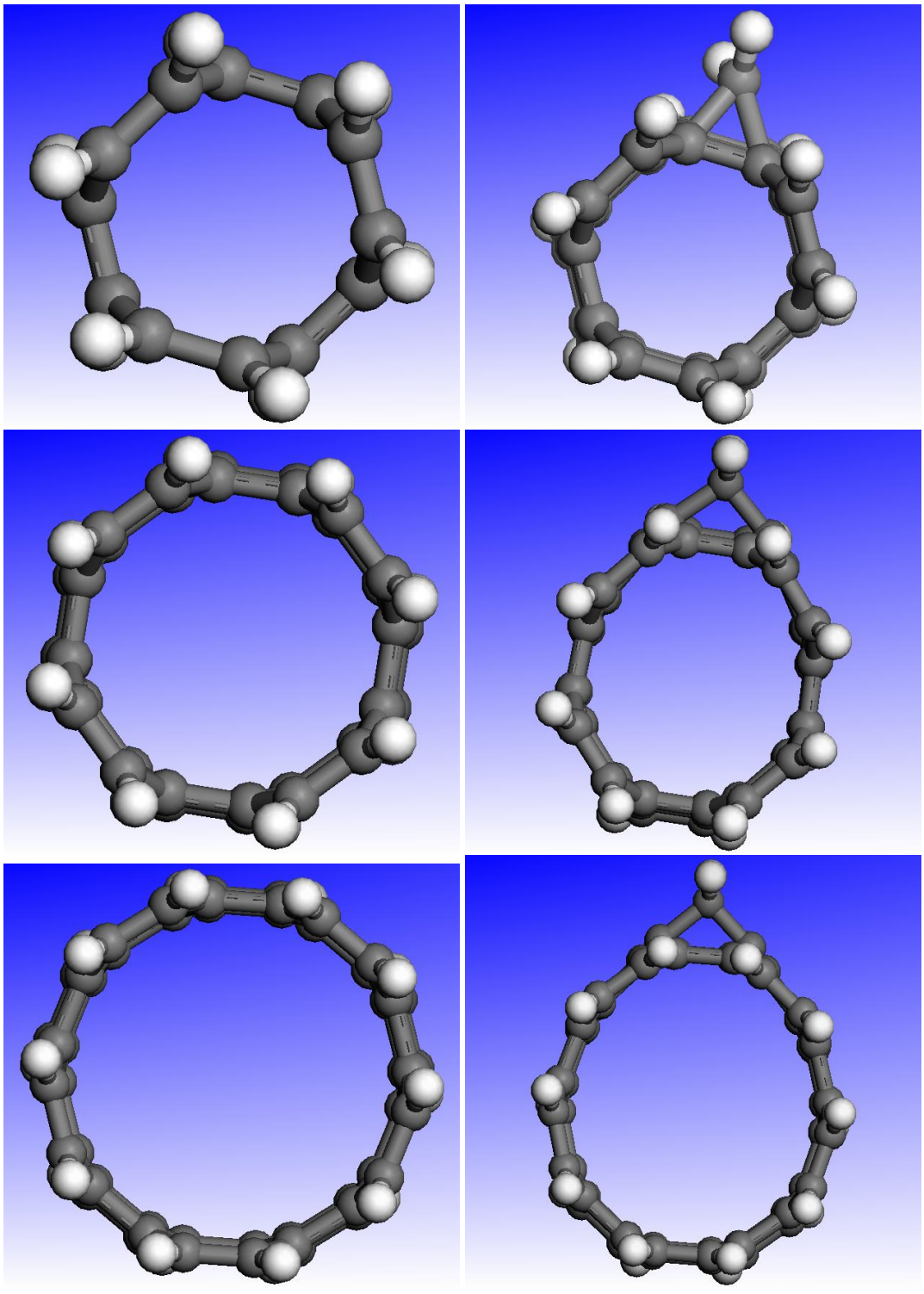
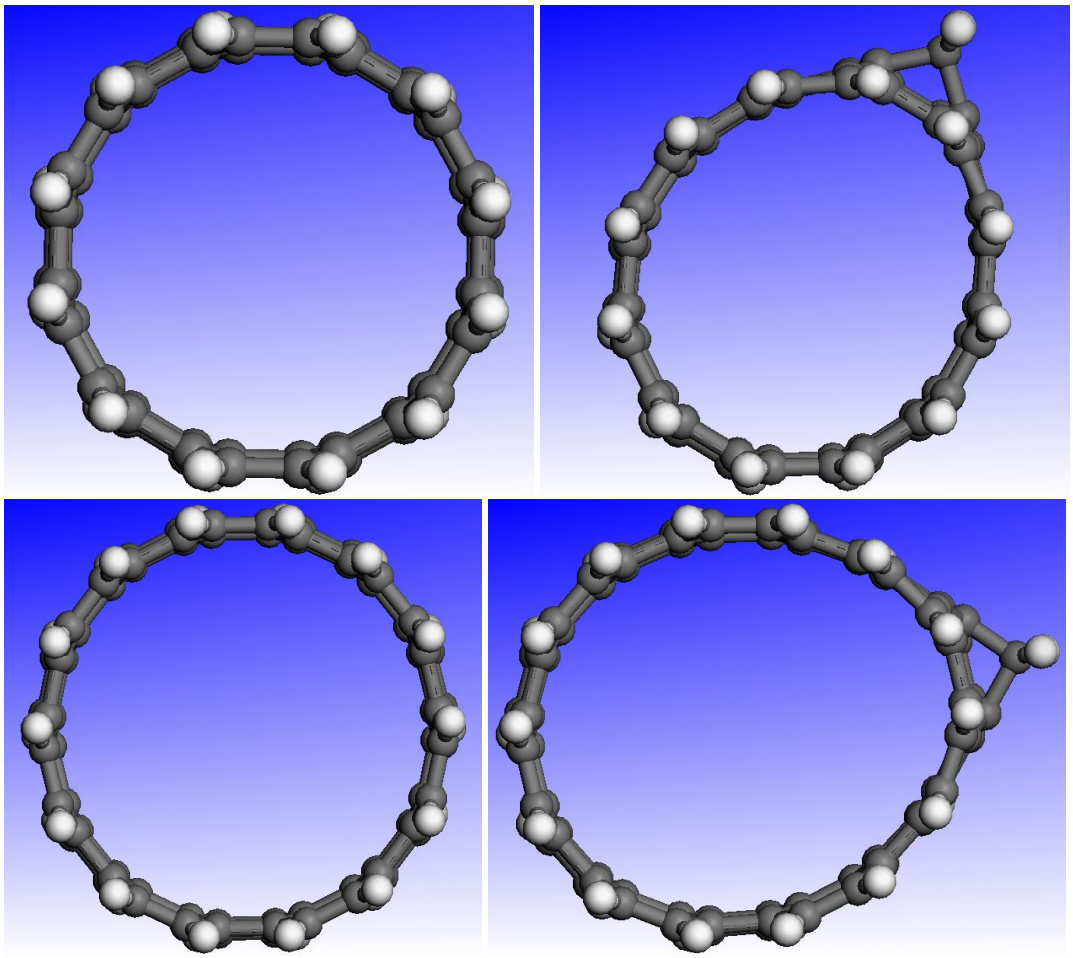


Figure S12 Variation of stability with diameter (Å)





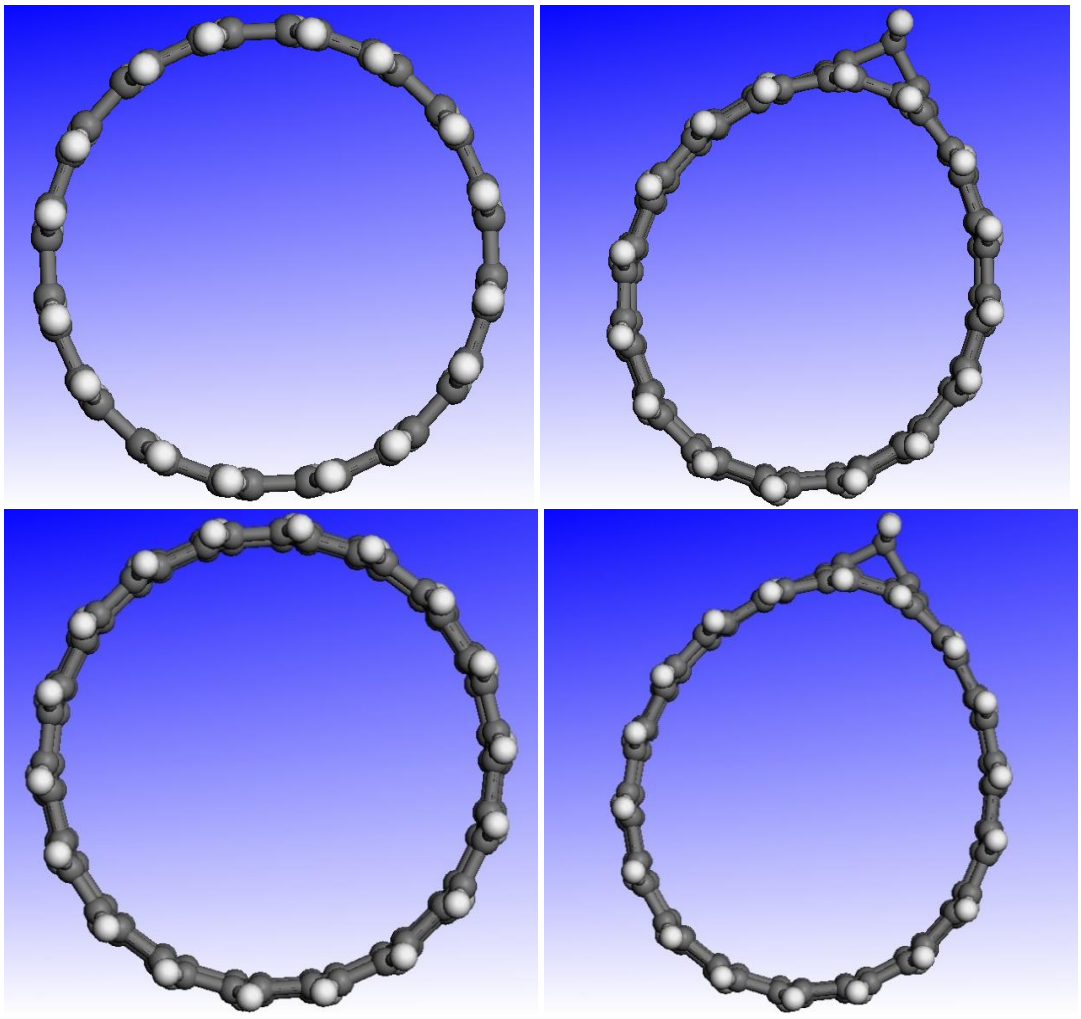


Figure S13 Optimized structures of SWCNTs of increasing diameter before (left) and after (right) methylene adsorption

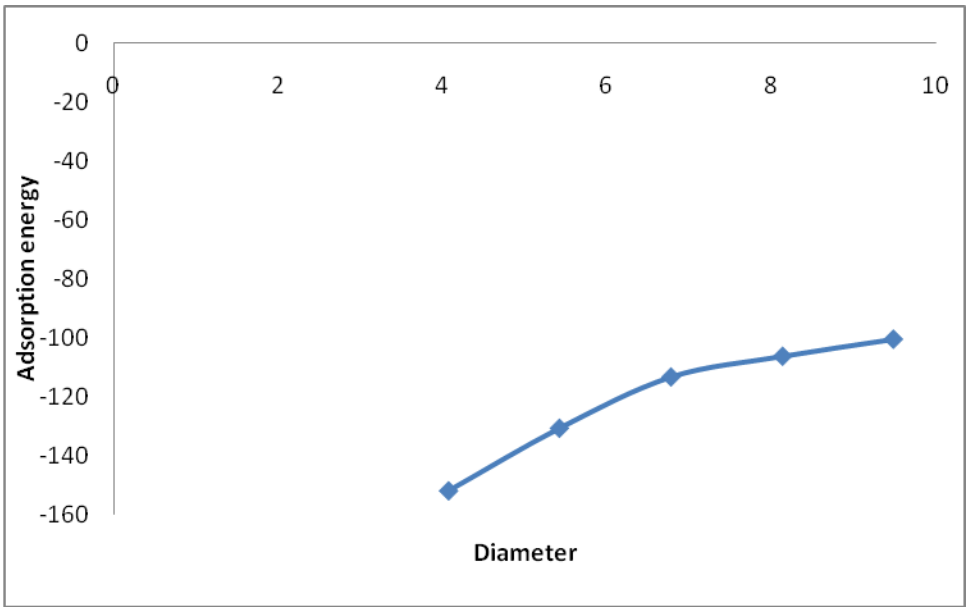


Figure S14 Adsorption energy of nanotubes of different diameters functionalized with methylene

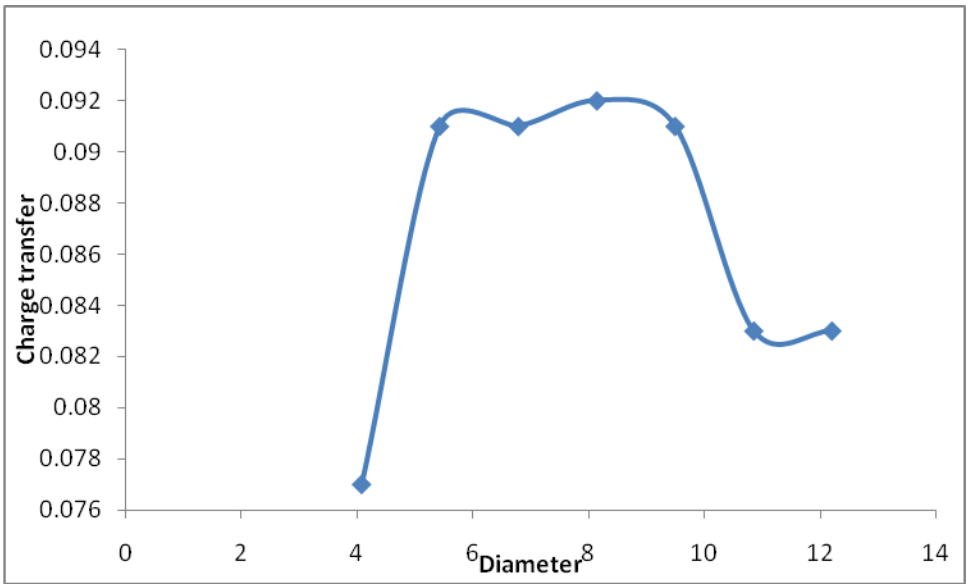


Figure S15 Charge transfer from the surface of nanotubes as a function of the diameter.

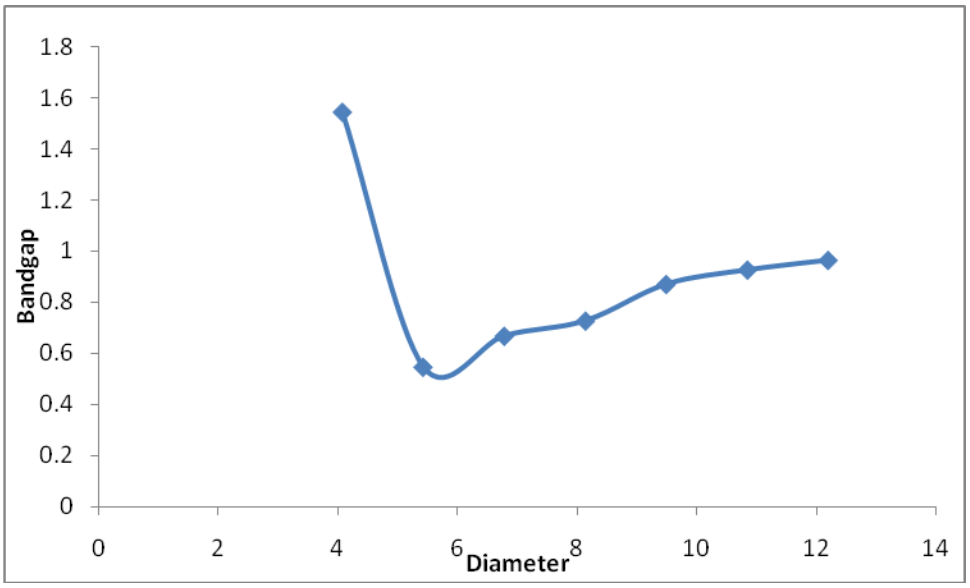


Figure S16 Bandgaps (eV) of nanotubes of different diameters