Edge Effect in Finite-length Pentaheptite Nanotubes

Noriyuki Mizoguchi

General Education and Research Center, Meiji Pharmaceutical University, Japan

Stone-Wales bond rotation[1] transforms four adjacent hexagons into two pentagons and two heptagons. Pentagon /heptagon defects may strongly affect the electronic properties of nanotubes. Crespi[2] applied the SW transformation to graphene in order to modify the hexagonal honeycomb lattice to form another lattice with only heptagons and pentagons (known as pentaheptite). A pentaheptite carbon nanotube PHCNT can be derived by rolling up pentaheptite layer. The one of main structural factors which determine the electronic properties of carbon nanotubes is the periphery structure of the hydrocarbons. It was found that zigzag edges in CNT raise the HOMO energy of the system (the edge effect). In this paper we theoretically study the effects of edges on the electronic properties of PHCNTs by using PM3 method.

We construct PHCNT with the units of azulen belt which is composed from azulene (a pair of pentagon and heptagon). Finite-length PHCNTs have the ends which are armchair edge or zigzag edge. PHCNT can be classified into the following three-types; (a) A-A type : the two ends are armchair edges, (b) Z-Z type : the two ends are zigzag edges, (c) A-Z type : one end is armchair edges and the opposite end is zigzag edges. The PHCNTs in Fig.1 are, from the left side, A-A type, Z-Z type and A-Z type.

We calculated the HOMO and LUMO energies of PHCNTs of the three types with various lengths and diameters. From the obtained results it is found that at each length in units of azulene belt, the HOMO energy for A-A PHCNT is lower than that for Z-Z PHCNT and the HOMO energy for A-Z PHCNT is in the midst of HOMO energies for A-A and for Z-Z PHCNT. This result means that the edge effect on HOMO energy found for pristine CNT holds also for PHCNT. However the edge effect on HOMO-LUMO gap is not found. The discrepancy between the edge effects on HOMO energy and on HOMO-LUMO gap in PHCNT is due to non-alternancy of the system.

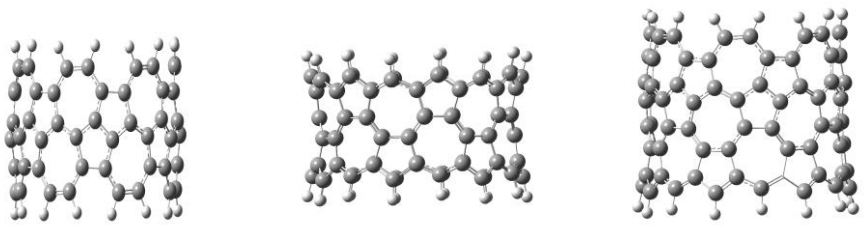

Figure 1 Three types of PHCNT; A-A, Z-Z, A-Z

[1] Stone A J, Wales D J *Chem. Phys. Lett.*, 501:128,1986

[2] Crespi V H, Benedict L X, Cohen M L, Louie S G *Phys. Rev.* R13303:B **53** 1996