

**MOLECULAR MODELING OF CARBON NANOTUBE  
JUNCTIONS**

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**ABSTRACT**

The structural and energetic properties of single-walled carbon nanotube junctions have been investigated theoretically. These junctions occur at the interface between two zigzag nanotubes having different diameters. One segment of the fused nanotube is fixed to the (5, 0) configuration, while the other segment is varied from (6, 0) to (10, 0). Practically, the junctions are constructed by inserting pentagon-heptagon (5/7) pair topological defects into the perfect hexagonal lattice. The study shows that the (5/7) pair defects are responsible for changing the electronic behavior of the proposed structure. HOMO and LUMO levels exhibit the even-odd “quantum size” oscillations which are functions of the diameter and the length of carbon nanotube junction. The energy gap indicates metallic or semi conducting behavior depending on both tube indices and tubule length. The low energy gap is the evidence that (5, 0)// (9, 0) 3UC SWCNTJ is a metallic tube. Furthermore, carbon nanotubes may be designed as a molecular rectifier by using donor and acceptor molecular sub-unit connected by a spacer. It shows that the (5, 0)// (7, 0) 3UC tube can be a possible structure of molecular rectifier diode because the HOMO energy level of donor, spacer and acceptor are sufficiently close to one another and the potential difference across the region is 0.199 eV. Therefore a single electron can travel from one side to another side.

**KEY WORDS:** CARBON NANOTUBS/ JUNCTIONS/ DEFECTS/ AM1/DFT