The regularities of p-electron conjugation in carbon nanotubes

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The axes of p_z-atomic orbitals coincide with normals to cylindrical surface consisting of carbon atoms. Thus the conjugation of p-electrons differs from conjugation of π-electrons in plane conjugated hydrocarbon molecules and singles out in special ρ-electron conjugation type [1]. Calculations of molecules modeling single walled carbon nanotubes (SWNT) (n,0) for n=6-9 were carried out for research of specific features of p-electron conjugation. The length of molecules was 12 hexagons placed on graphen surface along cylindrical axis of SWNT. The end carbon atoms were saturated with hydrogen atoms. Ab initio Hatree-Fock calculations were carried out in 3-21G basis set. The cylindrical stripes were selected in central part of molecules. The trans-carbon cycled chains were placed in those stripes. The number of chains m in cylindrical stripe ranged within 1-6 for each molecule. Electronic structure and band gap ΔE of molecules were calculated for optimized geometry conditions. Received results are presented in fig. 1.

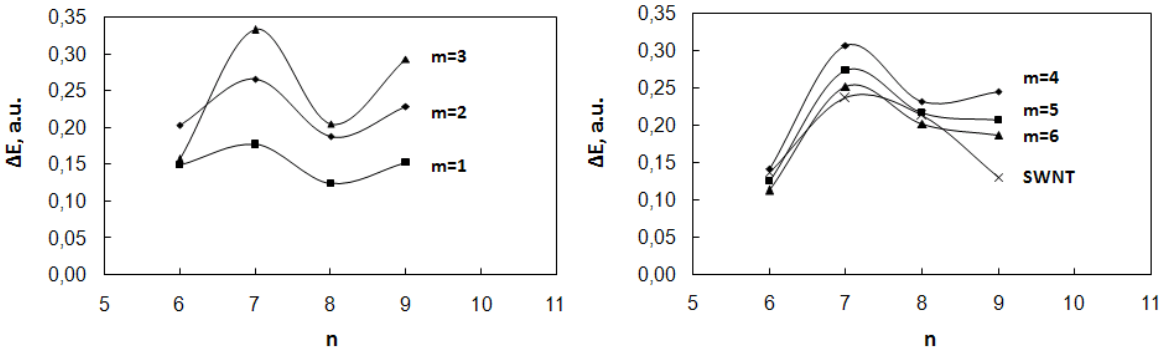

Figure 1: Dependence ΔE on index chirality n and number of trans-carbon chains m.

As follows from fig. 1 the band gap has oscillating behavior for trans-carbon chains for m=1-4. The maxima of amplitude agree with odd chirality index n. At the same time the oscillations for model molecule SWNT have minima in n = 3k. With further increase of m the character of band gap oscillations changes to SWNT oscillations. Thus, the p-electron conjugation corresponds to the combination of conjugation of p-electrons in cross-section SWNT and π-electron conjugation of cis-carbon chains placed on graphen surface in parallel with cylindrical axis of SWNT.

[1] D.A. Bochvar, E.G. Galpern, *Dokl. Akad. Nauk SSSR* **209**, 610 (1973).