Formation and electronic properties of defective carbon nanotubes. Theoretical approach

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Quantum chemistry research is presented of dehydropolycondensation mechanism of aromatic hydrocarbons in the presence of transition metals and their chlorides. Complexes consisting of benzene or naphthalene with a transition metal ion or chloride are chosen as model systems. It is shown that the metal ion weakens C-C and C-H bonds in hydrocarbons, at the same time complex anions present in the solution, absorb hydrogen. Thus dehydration of aromatic hydrocarbons originates with following polymerization in the orienting field of metal particles. Calculations show that the energy of interaction between transition metal ion and benzene ring is enough for bending of graphitic net with formation of closed graphite-like shells with metal inside. The results of calculations are confirmed experimentally, including formation of branched nanotubes[1].

Electron wave functions of the contact of semi infinite carbon nanotubes are calculated exactly using tight-binding model. Wave functions obtained are used to research scattering processes on the contact region. Volt- ampere characteristic of the contact is also estimated.

Program complexes Gamess, Hyperchem, Gaussian and programs developed by authors are used in calculations.

1. V.I. Kodolov, N.V. Khokhriakov, A.P. Kuznetsov, A.A. Didik, E.Sh. Shaiakhmetova, L.G. Makarova, E.G. Volkova, A.Yu. Volkov, V.L. Volkov. Methods of low-temperature synthesis and investigations of carbom metal containing nanostructures. Materials of Second International Symposium “Physics and Chemistry of Carbon Materials”. Alma-aty, Kazakstan, 18-20 Sept., 2002, PP. 298-301.