

ELECTRONIC STRUCTURE OF CARBON NANOTUBES OF VARIABLE DIAMETER

Popov A.P.*, Bazjin I.V., Smirnov D.S.

Department of education quality control,
Rostov State Pedagogical University,
Bolshaya Sadovaya Str. 33, Rostov-on-Don, 344007 Russia
E-mail: nanosys@mail.ru

Introduction

The creation of new nanoelectronic devices is not possible without using of elements with anisotropic conductivity. One of the ways to solve the problem is considered in the paper.

Results and discussions

The semi-empirical PM3-method [1,2] was used for the calculations of equilibrium configurations and electronic structures of carbon nanotubes of variable diameter, which can be obtained as the result of junction of (n,n) and (n,0) tubes along their common axis of symmetry. The belt of n 5-members and n 7-members cycles is appeared in the boundary of the junction (in the Figs 1-2 this cycles are shared out by the color).

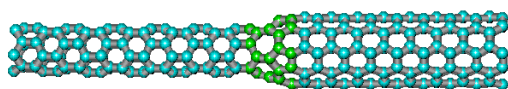


Fig. 1. Open tube (5,5)+(5,0) C₃₀₅

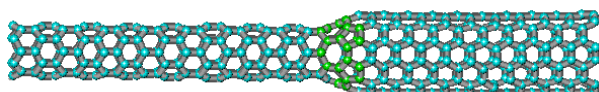


Fig. 2. Open tube (6,6)+(6,0) C₄₅₀

The lengths of bonds, full energy, heat of formation and any other characteristics were calculated for the equilibrium configurations of open and semi-open (5,5)+(5,0) and (6,6)+(6,0) nanotubes of variable diameter, in particular, there were found the energies of HOMO and LUMO orbitals and density of one-electron states.

We note above, that nanotubes of variable diameter can be considered as the result of junction of nanotubes with two different types of conductiv-

ity: metallic (n,n) nanotube and semiconductor (n,0) nanotube with width of forbidden gap about 0.5-1.5 eV. At the same time, as it follows from the results of calculations, the nanotubes of variable diameter are insulators with forbidden gap about 2.5-4 eV.

We consider also the nanotubes of variable diameter of such type as (n,0)+(n+1,0) (one of them is shown in Fig. 3). On the boundary between (n,0) and (n+1,0) tubes only one pair from 7-members and 5-members cycles is created. The axes of nanotubes, which take part in formation of junction, don't coincide, and as result the axial symmetry of construction at whole is absent.

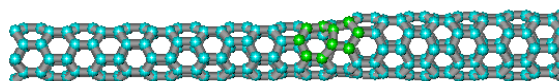


Fig. 3. Open tube (6,0)+(5,0) C₂₃₉

It's clear that nanotubes of variable diameter of such kind must possess anisotropic conductivity and therefore can be used as switching elements in future nanodevices.

Conclusions

The results of semi-empirical calculations show the possibility of existence of stable equilibrium configurations of nanotubes of variable diameter.

References

1. Stewart J.J.P., J. Comput. Chem., 1989, v. 10, p. 209.
2. Stewart J.J.P., J. Comput. Chem., 1989, v. 10, p. 221.