

THE INFLUENCE OF IMPURITIES AND DEFECTS ON ELECTRONIC STRUCTURE OF CARBON NANOTUBES

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Introduction

In the work systematic research of influence of impurities and defects on geometric and electronic structure of carbon zigzag and armchair nanotubes with using of semiempiric method of calculation is undertaken [1,2].

Results and discussions

In view of wideness of information connected with studying the influence of impurities (looks through the work [3]) on the geometry and physical characteristics of nanotubes here only a part of received results is discussed. Besides, special attention is given to defects as more widespread kind of infringement of regularity in arrangement of atoms of carbon in nanotubes.

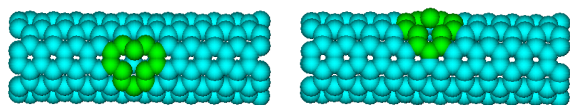


Fig. 1. In (6,6)-nanotube C_{264} one atom situated near the center of the tube is removed.

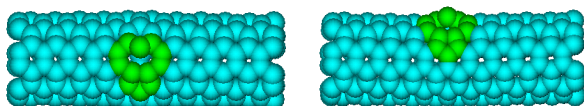


Fig. 2. After removal of an atom "defective" 5-members cycle is appeared.

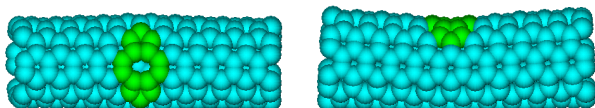


Fig. 3. After removal of two atoms of carbon two 5-members and one 7-members cycle is appeared.

In Fig. 1-3 the simplest samples of investigated defects is shown. It followed from the results of calculation that removal of one or just two atoms situated near the center of the tube doesn't lead itself to strong distortion of tube geometry. Considerable local tensions are appeared only in cases of chemical bonds formations. In spite of that formation of chemical bonds is energetically profitable, it is accompanied by local and sometimes global distortion of geometry of defective nanotube that is shown at the Fig. 3. However it is necessary to note that downturn of full energy is reached basically due to distortion of tube's geometry. The most interesting fact that sometimes occurrence of even single defect can sharply change not only size, but also type of conductivity of nanotube [4].

Conclusions

Done calculations point to the perspective of using nanotubes with defects in creation of nanodevices with set properties.

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.
3. A.H.Nevidomskyy, G.Csanyi, M.C.Payne, 2003, Phys.Rev.Lett., v. 91, 105502.
4. K.N.Nicolski, A.S.Baturin, V.S.Bormashov, *et al.* NATO Science Series, 2004, v. 172, 123.