ELECTRONIC STRUCTURE OF Y-JUNCTIONS OF CARBON NANOTUBES

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Introduction

In the work the calculation of electronic structure of number of the simplest Y-junctions in the frames of semiempirical PM3 is done.

Results and discussions

Methods of molecular mechanics [1,2] in the combination with semiempirical method of quantum [3,4] let to define equilibrium configuration and calculate electronic structure of number of the simplest Y-junctions of carbon nanotubes, which have slang name "twig". On the place of nanotubes conjunction defective cycles appear. Their type, number and mutual displacement can be enough various even in comparatively simple cases. In the Fig.1-2 the pair of topological nonequivalent Y-junctions of carbon (12,0)- and (5,0)-nanotubes, are shown.

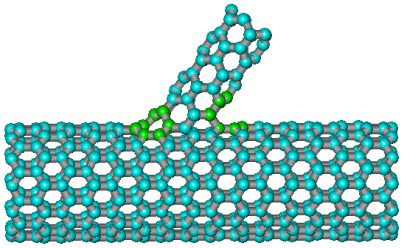

Fig.1. Y-junction (12,0)+(5,0) C_{433}

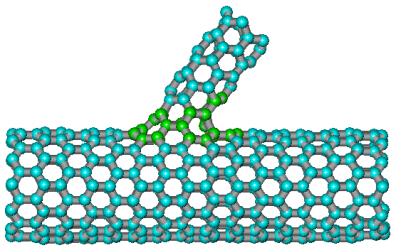

Fig.2. Y-junction (12,0)+(5,0) C_{435}

The length of bonds in the field of conjunction of nanotubes, heat of formation, full energy and electronic structure essentially depends on type, number and mutual displacement of "defective" cycles (colored in the pictures).

After the series of works [5-7] the possibility of working out the technology of synthesis of Y-junctions of carbon nanotubes became obvious though in the near future. Measurements performed in [5-7] show clearly the perceptivities of using them as switching elements of future nanodevices.

Namely in the connection with results getting by the authors [5-7] theoretical research of Y-junctions and ones of other types seems to be natural.

Conclusions

Equilibrium configuration of the whole series of topologically different Y-junctions of type "twig" is defined and in the frames of semiempirical method PM3 full energy and heat of formation is calculated and their electronic structure is also defined.

References

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