

ELECTRONIC STRUCTURE OF T-JUNCTIONS OF CARBON NANOTUBES

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Introduction

In the paper we continue the researches started in [1] where the possibility of existence of T-junctions of carbon (6,6)-nanotubes with monolayer of graphite was shown. Here some samples of T-junctions of carbon zigzag and armchair nanotubes were investigated.

Results and discussions

In the framework of semi-empirical method PM3 (worked out by Stewart [1,2] especially for calculation of electronic structure of carbon-contained organic molecules) the calculations of equilibrium configurations, full energy, heat of formation and electronic structure of different types of T-junctions of carbon zigzag and armchair nanotubes were done.

In the Fig. 1-3 only the part of researched junctions of type armchair + armchair, zigzag + zigzag and armchair + zigzag is shown.

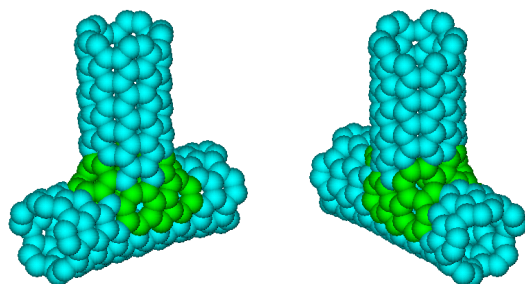


Fig. 1. T-junction C_{282} of type (5,5)+(5,5)

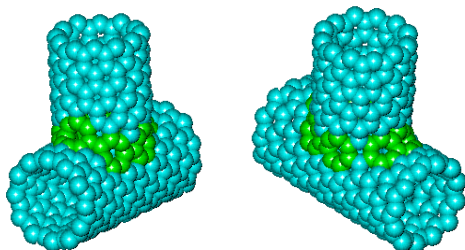


Fig. 2. T-junction C_{384} of type (10,0)+(10,0)

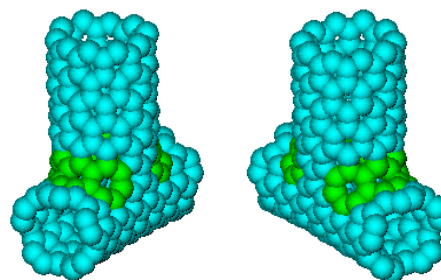


Fig. 3. T-junction C_{256} of type (5,5)+(10,0)

It should be noted we couldn't find stable configurations of zigzag + armchair T-junctions.

The results of our calculations are in good agreement in whole with published before in [4-6] results of theoretical and experimental researches of T-junctions.

Conclusions

In the frames of semi-empirical method PM3 the possibility of existence of T-junctions of carbon tubes of type armchair + armchair, zigzag + zigzag and armchair + zigzag, is predicted.

References

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