EXO-HYDROGENATED SMALL RADIUS ZIGZAG SWCNTs

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Introduction

Carbon nano tube (CNT) as a typical 1-D structure has some unique characteristics in electronic properties and physical features also. In particular, electronic behavior of small diameter CNTs are quite different from the properties of wide tubes just because of their strong "curvature effects" on π and σ bounds between carbon atoms [1, 2, 3].

In addition, clean energy industry is one of the promising applications of the CNTs (Hydrogen storage and Li- Ion batteries [4, 5]) and the motivation of this work is a systematic study of the curvature effects on the electronic and structural properties of narrow single wall CNTs (SWCNTs) after hydrogen adsorption.

Results and discussion

We have chosen zigzag (n, 0) SWCNTs with n=3, 5, 7, 9 (diameter range less than 7Å) and especially Fermi level "band gaps" have been under observation. Our results show that for SWCNTs with larger diameters the geometrical parameters like the C-C bound lengths and C-C-C bound angles are very close to their corresponding values in graphene sheet, so the curvature effects can be neglected surely, Fig.1 . On the other hand, after exo-hydrogenation, forming extra H-C bounds insert more confinements on the π bound electrons and therefore a clear band gap would be showed up in contrary to the expectations for these narrow tubes [6]. Because of narrowness of the SWCNTs, the case of indo-hydrogenation has not been under consideration. Fig.2 (left) shows the band structure of the (7, 0) SWCNT along its axes and in the right the Fermi area has been magnified.

Conclusions

By using DFT calculations (Espresso package) in our systematic study about narrow zigzag SWCNTs it is shown that the morphologic parameters for tubes with diameters larger than 7Å are very close to their value for graphene shit and therefore the curvature effects can be ignored in their studies.

In addition, after exo-hydrogenation and changing the sp^2 electronic hybridizations to the sp^3 one, the electronic band structures of the considered systems show a massive "Fermi level band gaps", Fig.3, which their widths increases with reduction of the tube's diameters, Fig.4. We have tried to justify this behavior of the band gaps by regarding the trend of bound angles variation.

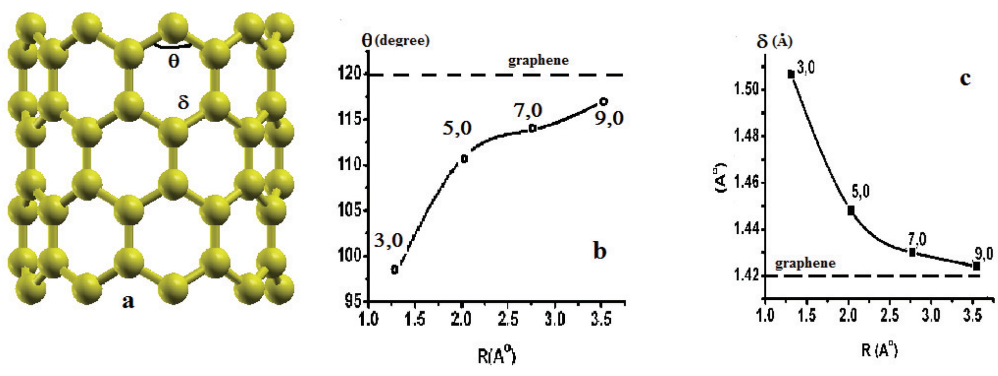

Fig.1 (a)- a zigzag SWCNT with specifying of ·θ and δ parameters; (b) & (c) - variation of the θ and δ parameters in terms of the tube's radii.

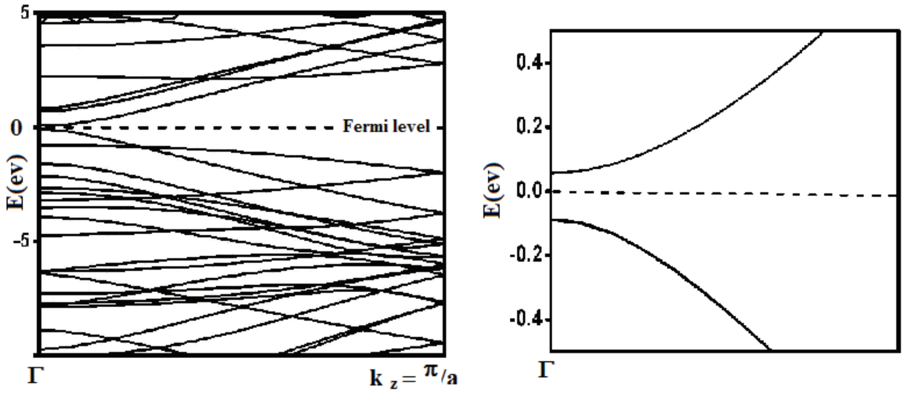

Fig.2 **Left**- Band structure of (7, 0) SWCNT; **Right**- Magnification of the Fermi level area in the left graph.

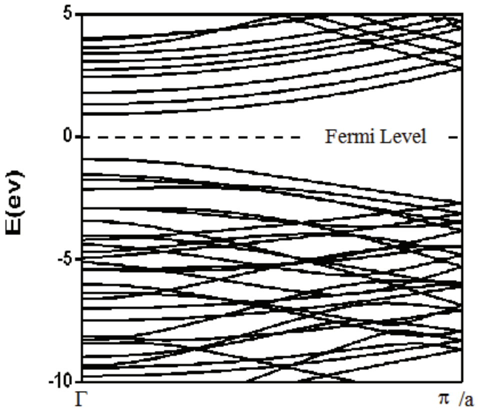

Fig.3 Band structure of the (7, 0) SWCNTs after hydrogenation.

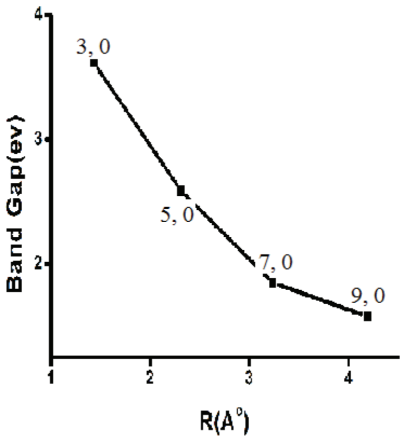

Fig.4 Variation of the band gaps after hydrogenation in terms of the tube's radii.

References

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