BOND ALTERNATION IN CARBON NANOTUBES

Poklonski N. A., Bubel' O. N., Kislyakov E. F,, Vyrko S. A.
Belarusian State University, Minsk, Belarus, pokIonski@bsu. by

The discovery [1] of superconductivity in 4 E single-walled carbon nanotubes raised a question about mechanism of this phenomenon. The knowledge of the precise atomic structure of carbon nanotubes of the smallest possible diameters is important in treating this question.

Contrary to the case of graphene sheet, where bond alternation is absent [2], one-dimensional structures are subject to Pierls distortions [3]. This phenomenon is well studied for the case of conducting polymers [4]. The possibility of Pierls distortions in carbon nanotubes was evident since very first work [5] predicting this new type of one-dimensional conductors, but quantitative estimate of this phenomenon is lacking till now.

We have performed semiempirical molecular orbital calculations of single-walled achiral carbon nanotubes with smallest possible diameters, namely zig-zag tubes (n,0), where n = 5... 10, and armchair (3,3), (4,4), (5,5). We employed modification [6] of MNDO program for infinitely long one-dimensional periodic structures. In all cases bond alternation were essential. The pairs (8,0), (4,4) and (10,0), (5,5) consist of the same amount of carbon atoms, but zig-zag and armchair tubes have different diameters and translation vectors along tube axis. For the same amount of carbon atoms armchair tubes is more stable than zig-zag (energy difference for (4,4), (8,0) pair is 87 kcal/mole).

Bond alternation was found to be large, especially for zig-zag tubes. In the case of (8,0) tube there are two types of bonds: double bond is 1,39 E, and single bond is 1,47 E. Along the circumference of the tube they are arranged in the same fashion as in the all *trcms*-polyacetylene.

In the armchair tubes bond alternation along the tube circumference is analogous to the cis-polyacetylene, being less in magni-

tude (1,42 E and 1,45 E for (4,4) tube) than in zig-zag ones. Arm-chair tubes are arranged so, that there is no bond alternation in *trans*-polyacetylene chains along tube axis, contrary to zig-zag tubes, where strong dimerization in c/s-polyacetylene chains along tube axis exists.

Nanotubes (6,0) and (5,0) show more complex atomic structure. In the case of (5,0) zig-zag nanotube there are short bond (1,40 E) and long bonds of different lengths, ranging from 1,43 E to 1,49 E. Short bonds are directed along tube axis.

In summary on the basis of semiempirical molecular orbital calculations we predict strong dimerization in single-walled carbon nanotubes in similar fashion, that is well known for poiyacetylene. It may be essential for explanation of conductive and other properties of carbon nanotubes.

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References

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