MODELLING OF GRAPHENE-NANOTUBE STRUCTURES: ARCHITECTURE, PROPERTIES AND APPLICATIONS

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New prospects related to the preparation and characterization of individual carbon nanotubes and graphenes (graphite sheets) have been currently developed in carbon nanotechnology during last years. The special graphene feature plays an important role in the electronic structure of carbon nanotubes (CNT) and graphene nanoribbons (GNR) whose conductivity type depends on the coincidence of the allowed wave vector with the Dirac points of graphene. CNT and GNR possess unique mechanic properties. That is why we began to study new symbiosis structures formed by CNT's and nanographenes/or GNR's [1].

We consider the reaction covalent addition zigzag (Z) edge or armchair (A) edge of GNR's to a single walled nanotube (SWNT) of different chirality. Between them more stable structures are Z-edged GNR covalent bonded (cb) with (n,n) SWNT's and A-edged GNR covalent bonded with (n,0) SWNT's. The covalent bonding change symmetry drastically both nanotubes and nanoribbons. Therefore, practically all cbGNR-SWNT structures are semiconductors. Each considered structure has "finger print" Van Hove peculiarities of electron spectrum similar separate SWNT's (or GNR's), and so they can be identified by Raman studies. We have studied free standing molecular bonded (mb) GNR -SWNT structures by molecular dynamic (MD) methods and showed that all nanoribbons align along nanotubes and take the form similar a part of cylinder. MD studies of considered quasi one-dimensional and two-dimensional cb-GNR-SWNT and mb-GNR-SWNT structures have showed high anisotropic elastic effects.

The calculations of reaction process were carried out in a single-determinant unrestricted Hartree-Fock approximation implemented in a semi-empirical version of the AM1 approach that is the most suitable for a thorough quantitative description of the odd-electron systems to which the above carboneous composites belong [2]. The calculations of electronic properties were made by DFT method using SIESTA program [3].

We have modeled also multi-terminal (T- and X- types) mb -GNR -SWNT junctions and their electronic properties. These junctions can be used as nanoelectronic elements with nonlinear current-voltage characteristics.

Some applications these structures (as components of elastic and conducting composites, optics and electronic elements, and so on) are considered.

This work was supported by Russian Fund of Basic Research (grant 08-02-01096) and Russian Academy Program № 27.

References:

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