Electronic waveguides and superlattices based on graphene with "lines" of chemisorbed hydrogen pairs

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New prospects related to the preparation and characterization of individual graphite sheets (graphenes) have been recently developed in carbon nanotechnology [1].

In this work, we predict by using DFT-LDA method a considerable transformation in the spectrum of graphene in the presence of periodically arranged lines of hydrogen chains at a distance of ~1 nm from each other. In the case of chemisorbed hydrogen chains on the graphene [2], conductivity of these "electronic waveguides" depends on the exact arrangement of hydrogen chains (similar to formation of spectrum of carbon nanotubes). We predict that these waveguides can have both pure metallic and semiconducting behavior.

It is possible to use the similar classification as in the case of carbon nanotubes. We consider only zigzag (n,0) and armchair (n,n) superlattices with different arrangement of H-pairs.

In the case of (n,n) superlattices, high density of states on a Fermi level is observed. It leads to pure metallic behavior in these superlattices in comparison with corresponding armchair nanotubes Since semiconducting (n,0) superlattices with different periods have different band gaps, it is possible to prepare complex systems like heterostructures. In this way, enclosing a metallic strip between semiconducting strips, we propose some electronic nanowaveguides, a one-atom thick nanowires. It has been considered also different 3-terminal junctions of the waveguides similar to Y nanotube junctions.

Our investigations show prospect of using considered based on the graphene structures in new nanodevices and integral nanoschemes [3].

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