Quantum dots based on graphane and graphane ribbons: structure and properties

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The emergence of graphene as a stable pure two-dimensional system [1] has been one of the most important events in electronic condensed matter physics over the laSt years. One of many interesting properties of graphene is the Dirac type of electronic band structure and the drastic changes of the conductivity of graphene-based structures with electron confinement. Thus, two possibilities for the realization of this effect have been realized: carbon nanotubes and graphene ribbons (GNR).

The GNRs are very interesting graphene successors. They have attracted much attention because of their properties and their potential for applications. In recent years GNRs have been experimentally obtained and theoretically investigated in details.

The total hydrogenation of graphene opens the dielectric gap in electronic band structure. The interface between hydrogenated and pure graphene shows the interesting quantum properties e.g. the confined graphene region in graphane shows the behavior of electronic structure like in quantum dots.

In this work the theoretical study of atomic structure and electronic properties of a quantum dots on graphane and graphane nanoribbons was carried out. The accurate theoretical approaches tight binding (TB) method and DFT were used for the description of the electronic properties of structures under study. The semiempirical tight binding scheme was chosen because it gives a good qualitative description along with high speed of calculation whereas DFT approach was used for verification of TB scheme. Using DFT method the quantum dots based on zigzag graphane roads and graphane nanoribbons with removed hydrogen atoms were investigated. The stability of the structures was analyzed and electronic properties (HOMO and LUMO levels) of the structures as well as dependence of the band gap upon the geometry of quantum dots were obtained.

[1] K.S. Novoselov, D. Jiang, F. Schedin, T.J. Booth, V.V. Khotkevich, S,V, Morozov, A.K. Geim, *Proc. Natl. Acad. Sci. USA* **102**, 10451 (2005).