Formation of quantum dots by "landing" of hydrogen atoms on graphene nanoribbons – modeling of process, structures and properties

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Recently, since pioneer work of 2008 of the Gaim and Novoselov group [1], even more often researchers have started to show steadfast attention to possibility of controllable creation GQD - a quantum “point” of graphene nanoislet [2-4]. This interest is connected not only with features of an electronic spectrum such nanoobjects, but also with an application wide field. Therefore there is a question - how most easily to generate GQDs with controllable properties?

Possible three simple schemes of experiments of controllable creation graphene quantum dots are offered [5,6]. Two of them are based on preparation of the bent surfaces which convex sites, as shown spent calculations, are favorable for adsorption of atoms of hydrogen: methods of “knife” action and “sinusoid” GNR under stress (Fig. 1).

The third technique of imposing of one layer of GNR array on another under certain angle [6] will allow to prepare GQDs in mass quantity (adsorption of H-atoms will lead to ribbon "splitting" on two zones: I – a free site from "mask" graphane type, and II – a site with one open party of be-grapnene, unprofitable for adsorption of hydrogen – see S4, Supplementary Online Material [7]).

Considered cases of favorable covalent bonding of H-atoms on specially prepared GNR places were modeled by a molecular dynamics method with use of package GULP. Energy spectra of the GQDs were calculated by tight-binding method within the limits of a software package dOXON with application periodic boundary which has shown earlier good coincidence of results to more exact *ab initio* calculations [8].

Examples of calculations the concrete GQD structures formed on the basis of usually received steady GNRs of type "zigzag" or "armchair", have shown basic possibility to vary size of a difference between bend gaps (HOMO-LUMO energy levels) from 0.1 eV to several eV with change of length of graphene nanosites (Fig. 2).

Let's notice also that schemes of the given experiments are certainly applicable and in case of use as the adsorbed atoms of fluorine (or oxygen), for creation ГКТ with nanosites of fluorine-graphene - FG (or oxide graphene - OG).

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References

[1] L. A. Ponomarenko, et al. Science 320, (2008) 356.
[2] S. Dreoscher, et al. H. Phys. Rev. B 84(2011) 073405.
[3] J. Lu, et al. Nat. Nanotech.6 (2011) 248.
[4] V, Gupta, et al. J. Am. Chem. Soc., 133 (2011) 9960.
[5] L.A. Chernozatonskii, A.A. Arthuch, D.G. Kvashnin, JETP. Lett. 95 (2012) issue 5.
[6] L.A. Chernozatonskii, A.A. Arthuch, D.G. Kvashnin, Appl.Phys. Lett. (2012) in press.
[7] D. C. Elias, et al., Science 324 (2009) 236.
[8] Xi Zhang, et.al, Nanoscale, 2 (2010) 2160.

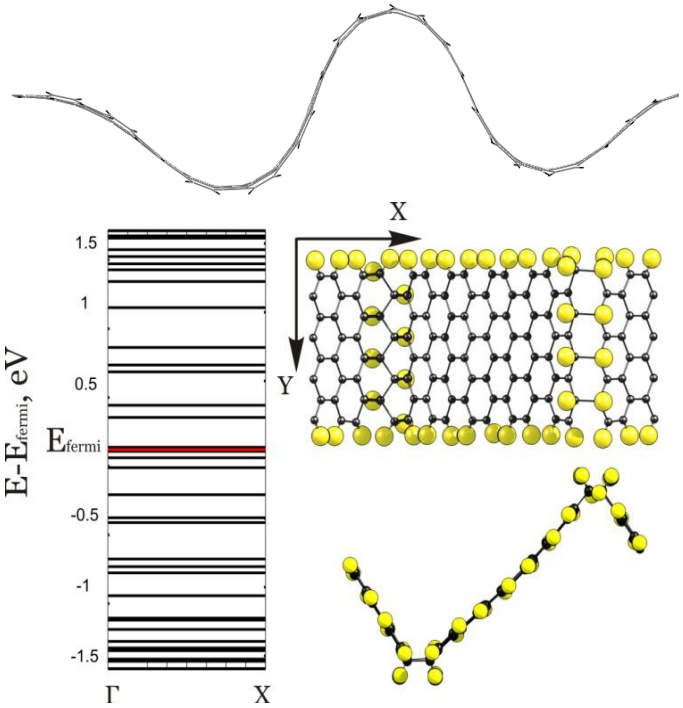

Figure 1. *The scheme of a sinusoidal bend of 8AGNR under its compression, and The GQD optimized structure - 64 sp2-carbon atoms between diamond-like C-H sites on the metallic 8AGNR (below on the right) and the spectrum of these superlattice (below on the left).*

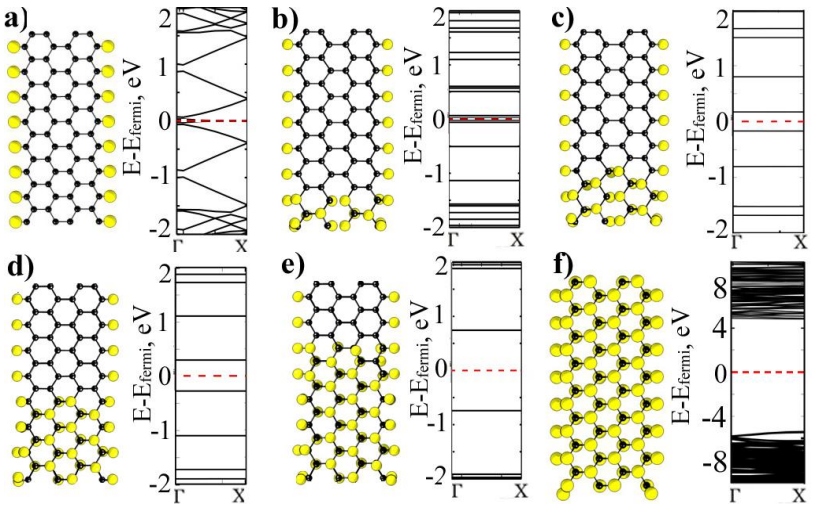

Figure 2. *Dependence of electronic properties 4ZGNR from concentration of the H-atoms adsorbed from two parties (yellow circles on schemes): change of a spectrum from continuous for "pure" GNR (a), «un-dispersive»*

spectra of quantum points with the growing forbidden zone (b-e), to a dielectric spectrum (f) – graphane nanoribbons at «full filling hydrogen » GNR. A dashed line – Fermi's EF level.