

Nanostructures based on H-(or F-) atom functionalized graphene elements for electronic and optic nano engineering

Chernozatonskii L.A.*¹, Artyukhov V.I.^{1,2}, Biro L.³, Mark G.³, Sorokin P.B.¹, Kvashnin A.G.¹, Kvashnin D.G.¹, Yakobson B.I.²

¹*Institute of Biochemical Physics, RAS, Moscow, 119334, Russia*

²*Rice University, Houston, Texas 77251, USA*

³*Research Institute for Technical Physics and Materials Science MTA, HAS, H-1525 Budapest, Hungary*

*e-mail: cherno@sky.chph.ras.ru

This report is review of experimental data and modeling (based on author papers) of main graphene nanostructures covered H (or F) prepared by special ways.

It is known hydrogenation (as well as fluorization) of graphene changes its electronic properties due to changing of sp² hybridization of C-atoms to sp³ one. Presence of the C-H regions can open the dielectric gap and organizes semimetal-like (M) or semiconductor (S) electronic waveguide paths (graphene nanopaths - GNPs) on this graphene sheet [1,2] and also organize graphene quantum dots (GQD) on graphane (or diamane - diamond-like nano thin films and nanoribbons) matrix [3,4]. We consider next main structures: 1) semiconductor superlattices of periodically changed graphane and graphene paths (or graphane pieces divided semimetal-like and semiconductor GNP); 2) arrays of individual graphene quantum dots (GQDs) on graphane matrix, and GQDs formed on graphene nanoribbons - GNRs; 3) modeling of mechanisms of formation of considered structures.

The electronic and mechanic properties of proposed structures studied by using *ab initio* (DFT) and molecular dynamics methods and compared them with the same properties of graphene-graphane (or graphene fluoride) structures. Possible ways of fabrication of nanoelectronic and nanooptics elements have been discussed.

[1] L.A. Chernozatonskii, P.B. Sorokin, J. Bruening, *Appl. Phys. Lett.* **91**,1831 (2007).

[2] A.K.Singh, B.I.Yakobson, *Nano Letters* **9**, 1540 (2009).

[3] V.I. Artyukhov, L.A. Chernozatonskii, *J. Phys. Chem. A* **114**, 5389 (2010).

[4] L. Chernozatonskii, P. Sorokin, A. Kuzubov, P. Avramov, A. Kvashnin, D. Kvashnin, B. Yakobson, *J. Phys. Chem. C* **115**, 132 (2011).