Nanomeshes based on BN-graphene bilayer

Demin V.A., Chernozatonskii L.A.

Emanuel Institute of Biochemical Physics of Russian Academy of Science, Kosygina st, 4, Moscow-119334, Russia
E-mail: victordemin88@gmail.com

Two-dimensional materials are attractive for different applications. The most famous 2D material – graphene. It has a lot of great properties as high strength and thermal conductivity, as well as the mobility of charge carriers. However, it has a significant disadvantage - the lack of energy gap, which make its use in electronic complicated. But we can change the electronic properties by creating a of holes [1,2,3], increasing of the layers number, their rotation relative to each other [4]. Another monolayer material - a hexagonal boron nitride, unlike graphene, has a wide band gap.

The DFT modeling of a two-layer material of graphene and hexagonal boron nitride - G-h-BN with periodically arranged holes presents in this work.

Both are single-layer material and have the same hexagonal lattice. Differences are the composition and lattice parameter (2.46 Ang in graphene and 2,504 Ang in boron nitride [5]). While layers are putting on each other, a disparity leads to the formation of structures such as moire patterns in bilayer graphene. Moire pattern consists of some areas as in AA- and AB- bilayered graphene, where it is possible to make holes. Structures, where one hexagon is removed from every layer and centres coincide, are consedered in this work. Features of the band structures of graphene nanomeshes exhibit in the electronic spectra bilayer nanomeshes G-h-BN, so they can have a wide range of electronic properties from metallic to semiconductor (Fig).

This work was supported by RSF №14-12-01217. The calculations were performed using resources of the Supercomputer Complex of MSU and the Joint Supercomputer Center of the RAS

[1] W. Oswald, Z. Wu, Phys. Rev., **85** (2012) 115431.
[2] L. A. Chernozatonskii, V. A. Demin, A. A. Artyukh, JETP Letters, **99** (2014) 309.
[3] D.G. Kvashnin, P. Vancsó, L.Yu. Antipina, G.I. Márk, L.P. Biró, P.B. Sorokin, L.A. Chernozatonskii, Nano Research (2014)
[4] S. Latil, L. Henrard, Phys. Rev. Lett., **97** (2006) 036803.
[5] A. Janotti and S.-H. Wei, Phys. Rev. B., **64** (2001) 174107.

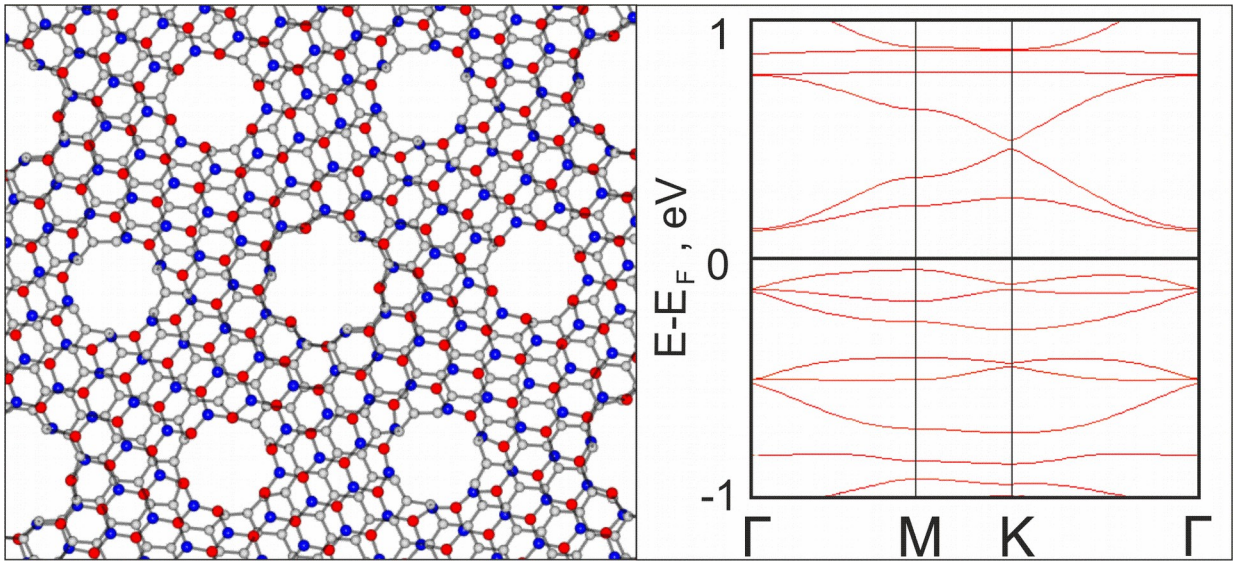

Fig. Semicoductor h-BN-graphene nanomesh and its band structure. E_g=0.18 eV