Nanocomposites and nanomaterials
Flexible 2D layered material junctions

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Two-dimensional (2D) materials commonly possess unique optical bandgap structures, extremely strong light–matter interactions, and large specific surface area. Graphene, hexagonal boron nitride and some transition metal dichalcogenides have emerged as promising building blocks for novel. nanoelectronics. They exhibit high carrier mobility, high on-off current ratio and excellent bendability that suit for future low-power consumption and flexible electronics [1]. These materials are laterally composed by strong covalent bonds, which provide great in-plane stability. Since the 2D materials are covalently bonded, the lateral heterojunction can only be formed by direct growth. These lateral heterojunction also exhibits intrinsic p–n junction behaviors such as rectifying properties and photovoltaic effects.

For extension of information about electronic properties of flexible lateral junctions based on graphene with different doping regions (Fig. 1) they will be calculated by us using such methods as electron density functional and first-principles pseudopotential on own program code [2]. For example, Fig. 1 demonstrates the charge regions of different densities for plane and curved lateral coplanar graphene/graphane heterojunctions, which can become the basis for creating a p-n junction, and the degree of bending to control its characteristics.

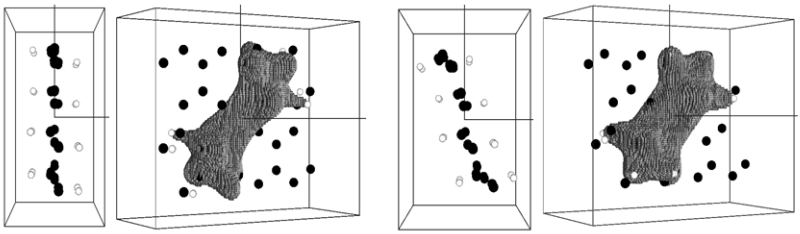

Fig. 1. Spatial distributions of the valence electrons density on the lateral (left – plane, right – curved) graphene/graphane heterojunctions within the interval of 0.6-0.5 of the maximum value

1. Li M. Y. et al. Heterostructures based on two-dimensional layered materials and their potential applications // Mater. Today.-2016.-19.-P. 323-335.
2. Ab initio calculation [E-resource]. – Access mode: http://sites.google.com/a/kdpu.edu.ua/calculationphysics.