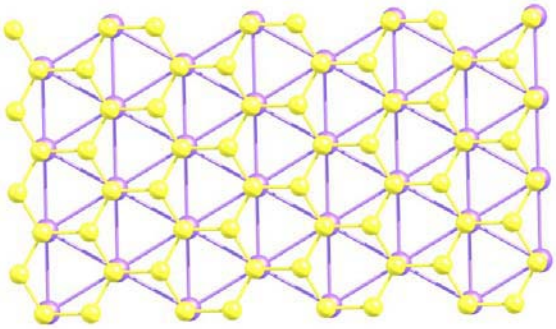
Structure, potential energy surfaces and electronic states of graphene- and multigraphene-based 2D extended complex nanocomposites

Avramov P.[*1,2,3], Sakai S.[1], Kuzubov A.[2], Entani S.[1], Matsumoto Y.[1], Naramoto H.[1]

[1]*Advanced Science Research Center, Japan Atomic Energy Agency, 2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan*
[2]*Siberian Federal University, 79 Svobodny, Krasnoyarsk 660041, Russia*
[3]*L.V. Kirensky Institute of Physics, SB RAS, Krasnoyarsk 660036, Russia*
**e-mail: paul@iph.krasn.ru*

The atomic and electronic structure and potential energy surfaces of 2D extended graphene- and multilayer graphene-based nanocomposites were studied using sophisticated *ab initio* Long-Corrected DFT (LC-DFT) technique. It was found that LC-DFT scheme coupled with periodic boundary conditions (PBC) allows one to calculate atomic structure of weakly bound multilayer graphenes and graphite with high accuracy. Using PBC and cluster approximations the potential energy surfaces (PES) of migration on and penetration through the carbon lattice of a set of adatoms (carbon, oxygen, nickel) were studied and a number of special points on PESes were found. It was found that LC-DFT scheme predicts the potential energy barriers of adatom migration on graphene surface with high accuracy.

Atomic and electronic structure and spin states of 2D extended complex graphene/Ni, bigraphene/Ni and trigraphene/Ni nanocomposites in all possible coordinations were studied using PBC DFT technique. It was found that eclipsed graphene/Ni coordination is energetically preferable (see Figure). The bi- and trigraphenes display AB and ABA stacking sequences coupled with small changes of interlayer distances in comparison with parent weakly bound multigraphenes. The spin states of graphene/Ni, bigraphene/Ni and trigraphene/Ni nanocomposites are determined by Ni substrates.



Atomic structure of 2D extended Graphene/Ni nanocomposite in eclipsed configuration.