

Electron and phonon characteristics of graphene, grafone and grafane structures

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Abstract: 1. Electron and phonon characteristics of graphene, grafone, and grafane have been investigated with the DFT method. Two configurations of the "boat" and "zigzag" type and three striped quasi-one-dimensional graphene-grafone periodic structures with different periods were modeled. The following stripes were considered: a row of carbon atoms comprises a hydrogen atom, the next carbon row does not comprise a hydrogen; two carbon atoms' rows contain several hydrogen atoms, the next two carbon rows do not contain hydrogen; six rows of carbon atoms contain hydrogen atoms, the next six rows do not contain hydrogen. 2. The interest in the striped structures have been arisen due to the possibility of creating two-dimensional electronic devices based on carbon films. The question of their stability is relevant, as on the borders of the graphene-grafone structures there is a change in the lattice parameters. As far as we know, such structures were not modeled before. 3. The properties of the studied electronic systems are listed below: • graphite is almost zero band gap; • grafone: the Fermi level is located on the slope of the peak in the hydrogen atoms' density of states, has the small band gap, shows the conductivity due the grafone hydrogen's orbitals; • B-type grafane has the band gap width of about 3 -3.5 eV; insulator; • striped graphene-grafone type 1 structure is the anisotropic conductor along the chains and presents conductivity both in the plane of carbon atoms and through the chains of the hydrogen atoms; • striped graphene-grafone type 2 structure is a poor conductor; • striped graphene-grafone type 3 structure is the anisotropic conductor along the chains and the insulator in the transverse direction. 4. The properties of the corresponding phonon systems are the following: • periodic graphene-grafone system and grafane have no imaginary frequencies; • striped graphene-type structure and type1 grafone have unstable phonon spectrum and contain two imaginary frequencies in the IR spectrum associated with the vibrations of the carbon atoms without hydrogen atoms; • striped graphene-grafone type 2 structure is also unstable on phonons; • striped graphene-grafone 3 structure is stable over the phonon spectrum. The results for the stripelined graphene – grafane structures are also presented.