Nanocomposites and nanomaterials

Wetting of graphene by methanol or water

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Graphene is a single-atom-thick sheet of sp^2-hybridized carbon atoms arranged in a hexagonal honeycomb lattice with a unique combination of properties. In spite of intense activity in graphene research, there are very few reports studying water (methanol) graphene interactions, which could be important if graphene is to be used in conformal coatings [1]. Motivated by this, we performed calculations of the energetic migration barriers of water (or methanol) on (or through) free-standed graphene sheets within the framework of the methods of the electron density functional and the ab initio pseudopotential. All calculations have been made with the proprietary source code [2]. The research object determined parameters of the superlattice and the atomic base. For simulation of the graphene plane that covered by water molecules (8% concentration steam) from two sides, the atomic base had 18 atoms. Figure 1 shows the change of the total energy of this atom system in the time of water molecules migration on graphene surface (energy is supplied in atomic units per atom, displacement - in Å). It shows this migration require the activation energy.

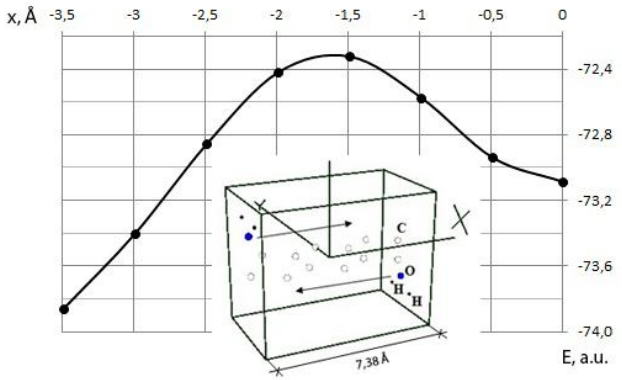

Fig. 1. The change of the total energy of atom system in the time of water molecules migration on graphene surface (energy is supplied in atomic units per atom, displacement - in Å).

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2. *Balabai R.M.*, Ukrainian Journal of Physics 58, 389 (2013).