The influence of the number of hydrogen atoms attached to naphthalene molecules on the potential barrier height

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Graphene is a promising material which allows to create a new class of electronic devices (carbon-based devices). Although nowadays graphene is mostly used as a passive element (as a simple conductive layer which does not contain logic elements) graphene is already considered as a real competitor to transparent electrodes made of indium oxide and tin oxide used in photovoltaic devices and displays on flexible basis [1-4].

Currently Langmuir-Blodgett method may be used to synthesize the graphene monolayers from the naphthalene molecules. The hydrogen atoms must be removed from the edges of naphthalene to form a graphene monolayer from the molecules of naphthalene. One of such technological methods based on raising the temperature or the action of the catalyst is described in work [5]. However, some of the hydrogen atoms can stay connected to the carbon atoms in naphthalene molecules. Therefore, this work is dedicated to the theoretical study of the influence of the number of hydrogen atoms attached to naphthalene molecules on the potential barrier height. This investigation is carried out for the detection of conditions for the formation of chemical bonds between the molecules of naphthalene with different numbers of hydrogen atoms. Energy potential barrier is formed when physical interaction between the molecules is becomes chemical interaction. Chemical bonds between atoms of the naphthalene molecules are formed as the result of overcoming the potential barrier between the molecules.

In this paper, investigation of dependence of the potential barrier height on the configuration of naphthalene molecules with different numbers of hydrogen atoms was carried out. Density functional theory with basis set B3LYP / STO-3g* with Lennard-Jones potential was used to perform numerical calculations. It was established that the smallest value of the potential barrier is achieved in the absence of hydrogen atoms in the naphthalene molecules. In this case, potential barrier height is equal of 0.01 eV. Consequently, the temperature of 48K is required for the formation of chemical bonds between the carbon atoms of different molecules of naphthalene with missing hydrogen bonds.

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