THE BEHAVIOR OF MESOGEN SYSTEM AT VARIATION OF GRAPHENE RIBBON SIZES AND VARIOUS IMPACTS

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Graphene has a great interest due to its electrical and thermoelectric properties. As noted in [1], the ratio between length and width of the graphene is strongly affected by these properties. The effect of the flow of nematic liquid crystals that we found (NLC) [2] on the graphene surface at the temperature changehad found its experimental confirmation in [3]. Therefore, it is necessary to consider the understanding of the influence of thegraphenesize and its type on the properties located on the surface of such electronic products as the NLC, when creating optoelectronic devices based on these compounds.

In this regard, the aim of this study was to research the influence of the size and type of graphene, the effects of temperature and electric field on the dynamics of nematic liquid crystals based on the arylpropargyl ethers of phenols. As a sample the nematic liquid crystal - phenylpropargyl ether of p-chlorphenol (PEC), located on the graphene in a planar orientation was used.

For the modeling of the behavior of these compounds we used the method of molecular dynamics based on the program GROMACS version 3.3.1 approaching liquid state. The performed experiments on computer modeling of the behavior of the polar PEC, located on the surface of grapheme ribbon, allowed identifying a number of laws. The little effect of the graphene ribbon type on the behavior of the NLC was shown. It was established that the ordering of nematic liquid crystals increase non-linear with increasing of the electric field. The determining role of graphene and the electric field on self-organization of the NLC in the enlightenment region was shown. It was found that in the area of enlightenment the ordering of the NLC starts to grow when the value of the ratio of width to length is 3: 1. This allows stating that at least two processes are taking place under the influence of temperature and electric field: First - "flow" of the molecules in the direction of X, the second - the rotation of the molecule in the direction of this axis. The second process may be due to the reorientation relative to the electric field of the molecules.

References:

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