Study of properties of liquid crystalline layers of selected cyanobiphenyls on surfaces of carbon and boron nitride nanostructures by computer simulations methods

Abstract

Composite materials based on liquid crystals and 2D materials such as graphene or hexagonal nitrogen boride are very interesting due to their practical application in optoelectronics, microelectronics and telecommunications. Their properties are largely determined by the interactions between the mesogen and the substrate, which are still not sufficiently studied at the molecular level. As part of the doctoral thesis, the properties of multilayer composites made of cyano-biphenyl located between graphene layers, hexagonal boron nitride or the surface of a bundle of single-walled carbon nanotubes were examined using computer simulations. Both the influence of the distance between the substrate surfaces and the effects related to the length of molecules from the cyano-biphenyl family were investigated.

The performed simulations showed the formation of clearly distinguishable, molecular mesogen layers, the thickness and order of which depend on the distance from the substrate. In addition, in the studied systems with molecules from a series of cyano-biphenyls, the occurrence of a phenomenon related to the length of molecules, the so-called odd-even phenomena. Molecules with an odd number of carbon atoms in the hydrocarbon tail show higher order than molecules with an even number. Increasing the distance between the substrate layers weakens the odd-even effects, which suggests that they are caused by interactions in the mesogen-substrate interface layer. Additionally, the odd mesogens in the series have a higher activation energy of thermal reorientation relaxation. From a practical point of view, it is also important to conclude that the polarization of the substrate (hexagonal boron nitride) significantly affects the structure of mesogen layers and accelerates the reorientation of molecules.