Nanoscale physics

Percolation threshold of n-Cyanobiphenyls mesogene phases between graphene – computer simulation study

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Properties of mesogene molecular structures are intensively studied because of fundamental scientific reasons as well as because of their vital potential applications in design of novel generations of displays and other opto-electronic devices [1].

Ordering of the mesogene layers anchored on different substrates strongly depends on substrate morphology and homogeneity [2]. Graphene is one of the most promising substrates due to its unique 2D structure and mechanical, electrical and optical properties. Aromatic nature of graphene and presence of two benzene rings in n-Cyanobiphenyls (nCB) structures lead to formation of planar alignment of anchored mesogene molecules.

nCB mesogene molecules located between graphene sheets form layered structures, that structural and dynamical properties depend on number of C atoms in the aliphatic tail of nCB as well as on the distance between the graphene sheets. Ordering effects and stability of mesogene phases were studied using molecular dynamics computer simulations. Effects of distance between graphene walls and mesogene surface density were investigated in the temperature range of 270 – 350 K.

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2. *Roscioni O.M., Muccioli L., Zannoni C.* Predicting the conditions for homeotropic anchornig of liquid crystals at a soft surface. 4-n-pentyl-4'-cyanobiphenyl on alkylsilane self-assembled monolayers // ACS Appl Mater Interfaces.-2017.-**9**, N 13.-P. 11993-12002.