On the ordering of n cyanobiphenyl mesogene molecules on graphene a computer simulation study

Wojciech Gwidzala, author

Abstrak

ABSTRACT
We studied ultrathin layers of 𝑛 cyanobiphenyl (𝑛 = 5,6,7,8) mesogene molecules forming thin films on a graphene plane using molecular dynamics simulations in a wide temperature range (220 420 K). Each modeled ensemble was heated to the maximum temperature and then cooled (reverse procedure). We calculated the second rank order parameter as a measure of the molecular order of mesogene molecules and we discuss the distribution of angles between them and the global sample director.