Nanostructured surfaces

Molecular dynamics of thin mesogene layer covering carbon nanotube

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Classical molecular dynamics simulations were performed for the thin layers covering the carbon nanotube. Two layers composed of n = 30 and n = 65 mesogenic molecules: 5CB, 6CB, 7CB and 8CB covering carbon nanotube were studied. We investigated the dependence of the dynamics of the mesogenic molecules of the temperature, since the simulations were performed for a wide range of temperature, from T = 210 K to T = 360 K. We study the dependence of the dynamics of the mesogenic molecules on the temperature. Several structural and dynamical characteristics of mesogenes were calculated: the mean square displacement, self diffusion coefficient, radial distribution function, activation energy, Lindemann index. Moreover, the comparisons of these characteristics with their counterparts of pure clusters (without nanotube) were done and are presented and discussed. The impact of the carbon nanotube on the mesogene clusters is clearly visible.

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