Nanostructured surfaces – POSTER PRESENTATION

Study of the dynamics of 5CB thin layer placed on the fullerene wall – computer simulations

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Classical molecular dynamics simulations were performed for a thin layer of 4-n-pentyl-4'-cyanobiphenyl (5CB) molecules placed on the fullerene wall.

The properties of 5CB molecules in such specific system was investigated by calculating several dynamical and structural observables (mean square displacement, diffusion coefficient, second order parameter, dipole moment autocorrelation function, etc.) which are discussed in this work.

We treated fullerene wall as infinite by applying two-dimensional periodic boundary conditions. The simulations were performed for six different temperatures (T = 240, 270, 300, 330, 360 and 390 K).

Some of the 5CB molecules from the layers tried to penetrate the fullerene wall by immersing themselves between the closest fullerenes.