Nanostructured surfaces

MD simulations of the dynamics of cholesterol molecules located between graphene sheets

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The cholesterol molecules, placed on graphene sheet, form a layer on its surface. In this work we have studied properties of two and three cholesterol layers placed between two parallel graphene sheets. The dynamics of such embedded cholesterol molecules has been studied at four temperatures.

Some dynamical and structural observables (mean square displacement, diffusion coefficient, radial distribution function and activation energy) were calculated and discussed. Moreover, we focus on the order parameters to check the capabilities of embedded cholesterol molecules to form cholesteric liquid crystals (chiral nematic phase).