Nanoscale physics

Properties of cholesterol – fullerene binary cluster: MD simulations

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The cholesterol is known as a constituent of several tissues in mammalian body. Out of necessity, the previous studies of the role of cholesterol focused on biological systems [1 -2]. However, it is less known that the cholesterol may exhibit interesting properties in other, non-biological systems.

In this work we investigate the cholesterol – fullerene binary cluster as well as a bulk sample, for comparison. Moreover, we solvate the system to assess the impact of water on the cholesterol- fullerene cluster. The systems were investigated at four temperatures (T = 280, 295, 310 and 325 K)..

By analyzing the dynamical and structural observables (mean square displacement, diffusion coefficient, radial distribution function and activation energy) we discuss the behavior of cholesterol molecules in the such specific, non-biological environment.

[1] *Gburski Z., Gorny K., Raczynski P.,* The impact of a carbon nanotube on the cholesterol domain localized on a protein surface// Solid State Communications -2010.-**150**.-P. 415-418.

[2] *Raczynski P., Gorny K., Samios J., Gburski Z.,* Interaction Between Silicon–Carbide Nanotube and Cholesterol Domain. A Molecular Dynamics Simulation Study// J. Phys. Chem. C. -2014.-**118**.-P. 30115–30119.