Nanoscale physics – POSTER PRESENTATION

Molecular dynamics simulations of the dynamics of small cholesterol systems

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The role of cholesterol and its properties in biosystems are well known. Although the excess of cholesterol may prove unhealthy, it is needed in human body, for example for proper functioning of cells membranes.

In our previous studies we widely investigated the properties of cholesterol in various systems, e.g. we investigated the process of extraction of cholesterol molecules from the small deposit located on protein surface by nanotubes [1]. Unfortunately, we have never studied the behavior of cholesterol in small systems, just such we placed on protein surface in [1].

In this work we investigate two small cholesterol systems composed of 15 and 30 molecules. The water is ubiquitous in all biological systems, thus all simulations were performed in water environment. Moreover, to examine the impact of water of the cholesterol systems we compare the obtained results with the similar nonaqueous samples. Four temperatures, including physiological, (T = 270, 290, 310 and 330 K) were taken into account.

By analyzing the dynamical and structural observables (mean square displacement, diffusion coefficient, radial distribution function and activation energy) we discover the impact of water and the behavior of cholesterols in such a small systems.

[1] *Raczyński P., Górny 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.