Nanoscale physics

The computer 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.

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 the water environment. Moreover, to examine the impact of water of the cholesterol systems we compare the obtained results with the similar nonaqueous samples. The simulations were performed at four temperatures, including physiological, (T = 270, 290, 310 and 330 K).

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