Nanoscale physics – ORAL PRESENTATION

Molecular dynamics simulations of the nanoindentation of biomembrane by carbon nanotubes of a different chirality.

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The process of nanoindentation of phospholipid membrane by the carbon nanotubes of a different chirality was studied using steered molecular dynamics method. The phospholipid membrane protects the interior of the cell for external molecules, proteins and particles. It is a challenging task to find nanoobjects, which are capable to deliver cargo (for example drugs) to cells *via* phospholipid bilayer, without damaging its structure.

Three nanotubes of the different chirality were used (7, 7), (10, 10) and (12, 12). The nanotubes were pushed through the phospholipid bilayer with constant speed. Three different pulling velocities were studied: 0.5, 1.5 and 2.5 m/s. All simulations were performed at the physiological temperature 310 K and in water environment.

The force acting on nanotube during membrane indentation, work and free energy changes were calculated and are presented and discussed.

A series of simulations of pulling carbon nanotube out of the bilayer were also performed. Carbon nanotube cannot permanently damage the structure of phospholipid bilayer due to protective functions of membrane. In that work we also analyze the damages caused during nanoindentation process for potential use the nanotubes as a containers to drug delivery.

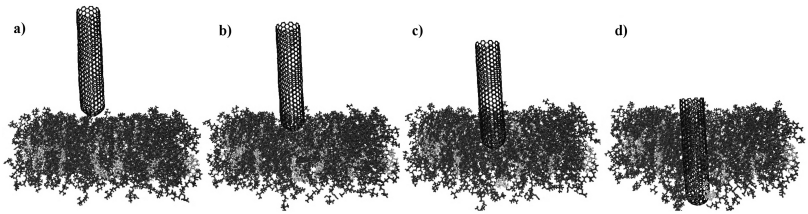

Fig. 1. Snapshots of the phospholipid bilayer penetration by carbon nanotube for four penetration depth.