سمینار هفتگی ماده چگال نرم

عنوان سمینار

A study on the process of passive uptake of nanoparticles by coarse-grained MD simulation

ارائه دهنده

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چکیده

The aim of my thesis is to investigate the passive wrapping of nanoparticles by a lipid membrane in the uptake process using molecular dynamics computer simulations. The simulations are carried out by the Virtual Cell Model (VCM) software package, a computational framework that creates a large scale coarse-grained multi-component cell model developed by Prof Mohammad Reza Ejtehadi's Soft Matter Group at Sharif University of Technology. VCM can model the dynamics of different parts of the cell and investigate their mechanical properties.

In our model, the membrane is represented by nodes that are on a closed triangular mesh network with bending rigidity between adjacent triangles and harmonic springs between connected nodes. The fluid-like behavior of the membrane (Which is caused by the diffusion of lipid molecules on the surface of it) is mimicked by changing the structure of the node connections. The mechanical energy of the membrane is minimized through a Monte Carlo selection of the best network configuration of triangles through the course of the simulation. The nanoparticles are simulated as very rigid membranes that have a constant shape (polyhedral) and network throughout the simulation.

The results show that membranes that mimic fluid-like behavior have a higher chance to wrap the nanoparticles compared to membranes that only have elastic properties. As a result of minimizing the total free energy of the system, multiple nanoparticles attached to the inner wall of the membrane, are guided to each other to reduce the overall bending energy of the membrane wall. We were not able to observe vertical tubular-shaped protrusions in our membrane model which has been previously reported in the literature. However, we showed that in our simulations nanoparticles that create small clusters can result in lateral tubular-shape protrusions.

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