Lipid bilayer interacting with nanoparticles of various values of hydrophobicity

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Abstract

Self-assembled lipid bilayers are the protective barrier of living cells, which prevent passage of high molecular weight components, including ions, proteins, but allow for exchange of substances and information between the cell and its surroundings. A challenging problem is raised for translocation of drugs, nanoparticles, genes through lipid bilayers. As it is difficult to obtain microscopic information of nanoparticles interacting with lipid membranes in experiments, there is still missing knowledge about the mechanism of translocation processes. This concerns in particular passive transport which does not involve consumption of energy such as ATP-hydrolysis.

We implement a simplified version of MARTINI model for DPPC[1] to construct lipid membrane interacting with nanoparticles (NPs) of different numbers (50, 100) and various values of hydrophobicity, H. Our interest lies in the general physical mechanism of passive translocation of particles through self-organized amphiphilic membranes and their impact on the other membrane-properties such as the relationship between permeability of membrane and the level of hydrophobicity of NPs is investigated. We demonstrate that nanoparticles having a specific hydrophobicity enhance the permeability of water through the membrane. Umbrella sampling simulations are conducted to study the free energy landscape of NPs with respect to the distance from the membrane including the internalized states. In a certain range of parameters we could study the translocation processes directly.

References:

1. S. Marrink et al., J. Phys. Chem. B 108, 750-760 (2004).