Diffusive translocation of nano-object through model lipid bilayer membranes

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Abstract

Self-organized lipid bilayer membranes (LBM) have been studied using the bond-fluctuation method with an explicit solvent model. The LBM represents a potential barrier with respect to nano-objects such and polymer chains or nano-particles which is controlled by the relative hydrophobicity of the interacting objects. We have shown that homopolymers consisting of repeat units with a balanced hydrophobicity show the signature of critical adsorption with respect to the membrane at a relative hydrophobicity of about $H_C \simeq 0.67$ which is above the threshold of an ideal penetrable membrane, where H=1(0) corresponds to fully hydrophobic (hydrophilic) units. This can be explained by a free energy barrier caused by the insertion of monomers into the ordered LBM. As a result the potential profile the LBM exhibits an attractive (surface) part which leads to more complex adsorption scenarios of the homopolymer chain. Close the critical point of adsorption the polymer chain can undergo a diffusive translocation through the membrane which is in accordance with the mean first passage time calculated from the free energy profile of the chain. Related with diffusive translocation of the chain enhanced solvent permeability is observed. Furthermore, we have studied the interaction of small nano-particles (NP) with the LBM. Similar to the results obtained for homopolymer chains the permeability of NP displays a maximum close to 0.67. At this degree of relative hydrophobicity the NPs form aggregates in the aqueous phase which cause some cooperative effects of their translocation behavior which is responsible for a shift of the translocation threshold towards higher values of *H*. Patchy NPs, which consist of a hydrophobic and hydrophilic units display a similar behavior. In this case stronger surface localization and reduced permeability is observed, while aggregation is suppressed. Solvent permeability is correlated with adsorption of NPs at the membrane as for the case of polymers. Our studies reveal a novel diffusive pathway of translocation of nano-objects through LBM controlled by a balance of hydrophobicity. Perturbation of the membrane close to the adsorbed objects causes enhanced permeability of solvent molecules[1,2].

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