# Monte Carlo study of the influence of polymer chains on the permeability of lipid bilayers

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## Abstract

It is known from experiments [A. L. Lynch et al., Biopolymers 31, 6096 (2010)] that the permeability of lipid bilayers for small molecules may be influenced by polymers depending on their hydrophobicity. This effect may have various medical applications such as drug delivery or conservation of blood. However, the mechanism of polymer-induced permeability is not known. Within the framework of the Bond Fluctuation Method we model amphiphilic lipids embedded into an explicit solvent, where we mediate the hydrophobic effect by short-range repulsive interactions. This model reproduces self-organized lipid bilayers and polymer chains on a coarse grained level under variation of the hydrophobicity of the chains. As an effective measure for the disturbances of the bilayer induced by the chain we analyze the permeability of the membrane with respect to solvent molecules. A hydrophilic chain stays in a non-adsorbed state in the solvent phase and has no significant influence on the membrane-permeability. On the other hand, a hydrophobic chain is strongly adsorbed to the membrane and gets trapped within the hydrophobic layer. In this case, the permeability with respect to the solvent is reduced locally (see Fig. 1). For intermediate hydrophibicities we see a transition-state, where the chain shows spontaneous adsorbtion and desorption events and is able to translocate though the membrane. The local solvent-permeability of the membrane has a maximum near this transition-state which indicates a strong distortion of the bilayer configuration close to a translocating chain.

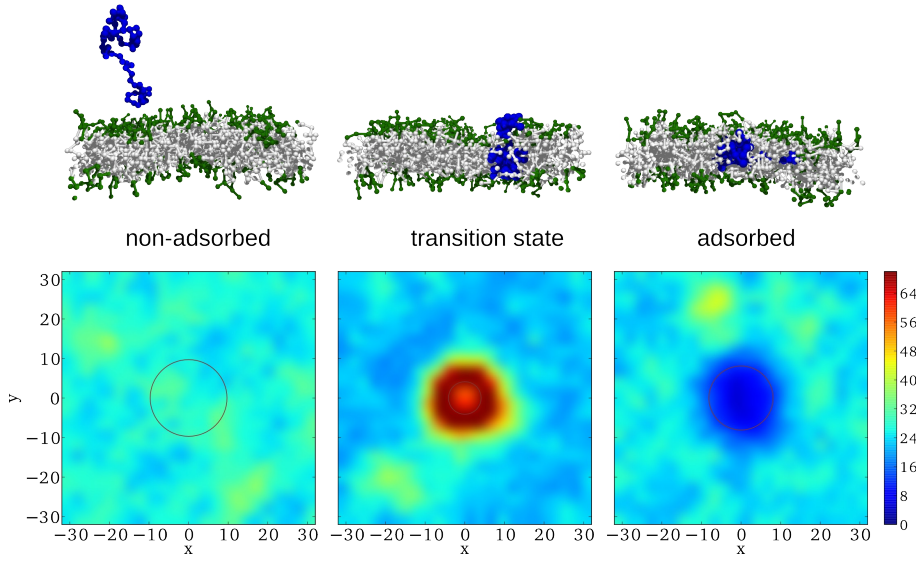


Fig. 1. Solvent-permeability of a lipid bilayer interacting with polymer chains of various hydrophobicity. Simulation results are shown for a hydrophilic chain (non-adsorbed), hydrophobic chain (adsorbed) as well as a chain near the transition state. The coordinates x and y denote the distance from the chain projected to the bilayer-plane.