

## Theory and Simulation of Homopolymers Interacting with Lipid Bilayers: From Critical Adsorption to Pore Formation

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### Abstract

We consider the interaction of homopolymer chains and lipid bilayer membranes as a function of the polymer's hydrophobicity. In this talk, results from coarse-grained Monte Carlo simulations are compared to the predictions from the Edwards Model for ideal chains in an idealized potential model. There is an adsorption transition of the polymer at the bilayer—solvent interfaces close to a balanced value of polymer hydrophobicity [1], where the membrane becomes energetically quasi-transparent for the polymer. An increase of translocation frequency of the polymer through the membrane is expected close to the balanced point according to the Edwards Model in agreement with simulation results. Simulation results further suggest that a polymer close to the transition point assumes a globular state. During polymer translocation, a transient pore is formed, which hosts the globule. When located in the bilayer's core, the polymer globule can be considered as a first approximation for a transmembrane protein effecting facilitated passive transmembrane transport [2]. In particular, close to the interface between globule and lipid tail phase, simulation results show an enhanced porosity of the membrane by means of small spontaneous pores allowing for solvent translocation. A possible link between polymer-induced permeability at a balanced hydrophobicity and the enhancement of fluctuation induced lipid ion channels close to the main transition temperature of a lipid bilayer is discussed [3].

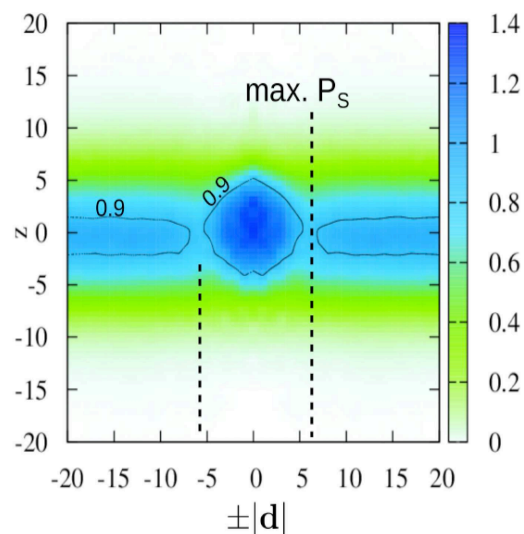


Fig. 1: Effective permeability barrier for solvent as given by the sum of lipid tail- and polymer volume fractions. The volume fraction is given relative as compared to an unperturbed bilayer's core as a function of the projected distance,  $d$ , from the polymer center of mass, and the distance,  $z$ , from the bilayer's mid-plane. A maximum solvent permeability ("max.  $P_s$ ") is observed at a distance  $d$  denoted by dashed lines.

[1] J-U Sommer, M Werner, V Baulin, *Eur. Phys. J* **98**(1), 18003 (2012)

[2] H Rabbel, M Werner, J-U Sommer, *Macromolecules* **48**(13), 4724-4732 (2015)

[3] T Heimburg, *Biophys. Chem.* **150**, 2-22 (2010)