

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/309135708>

# Spontaneous curvature of biomembranes from molecular simulations

Poster · September 2016

CITATIONS

0

READS

86

2 authors:



[Bartosz Różycki](#)

Institute of Physics of the Polish Academy of ...

38 PUBLICATIONS 684 CITATIONS

[SEE PROFILE](#)



[Reinhard Lipowsky](#)

Max Planck Institute of Colloids and Interfaces

472 PUBLICATIONS 17,327 CITATIONS

[SEE PROFILE](#)

Some of the authors of this publication are also working on these related projects:



Membrane curvature generated by layers of ions, small molecules, and nanoparticles [View project](#)



Intrinsically disordered linkers in multi-domain carbohydrate-active proteins [View project](#)

## Abstract

Biomembranes are usually asymmetric in the sense that their two leaflets differ in their lipid composition. In addition, the two sides of the bilayer membranes are typically exposed to different aqueous solutions. Because of these asymmetries, the membranes prefer to curve in a certain manner as quantitatively described by their spontaneous curvature, see Fig. 1. We consider solutions of 'particles' that form adsorption or depletion layers in front of the membrane leaflets. The particles considered here are water-soluble, have a size between a few angstrom and a few nanometers as well as a rigid, more or less globular shape, and do not permeate the lipid membranes. Examples are provided by ions, small sugar molecules, globular proteins, or inorganic nanoparticles with a hydrophilic surface. We use analytical calculations and coarse-grained molecular dynamics simulations to study how the spontaneous curvature of lipid bilayers is induced by the adsorption and depletion layers of such particles.

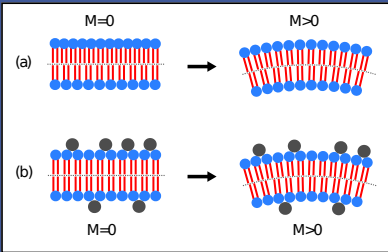


Figure 1: Two molecular mechanisms for bilayer asymmetry: (a) different lipid densities within the two leaflets and (b) different adsorbate densities at the two head-group layers.

## DPD simulations

Dissipative particle dynamics (DPD) is a coarse-grained molecular dynamics technique with explicit solvent and local momentum conservation [1]. Our DPD model includes water, lipid molecules as well as adhesive and non-adhesive particles. Small water volumes are represented by single beads of type W. The water-soluble particles are represented by single beads of type P. A lipid molecule consists of three hydrophilic H beads and two hydrophobic chains, each consisting of six C beads [2,3]. The diameter of the beads is  $d \approx 0.8$  nm. The density of the W beads is such that the normal pressure  $P_N$  is equal to the pressure of pure water at standard DPD conditions. The key quantities that are monitored in the simulations are the density profiles of the DPD beads and the membrane lateral stress profile  $s(z) = P_N - P_T(z)$ .

## Membrane tension

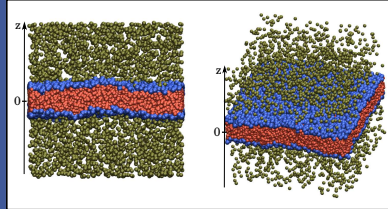


Figure 2: Lipid bilayer exposed to water-soluble particles. The C, H and P beads are shown in red, blue and tan, respectively. The water beads are not shown. Because of the periodic boundary conditions, both leaflets of the lipid bilayer are exposed to the same environment.

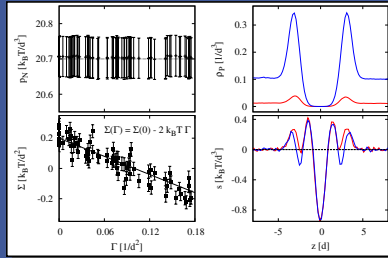


Figure 3: Symmetric adsorption of particles on a symmetric bilayer membrane. (Left) Membrane tension,  $\Sigma = \int s(z) dz$ , decreases with the leaflet coverage by the adhesive particles,  $\Gamma = \frac{1}{2} \int [\rho_P(z) - C] dz$ , according to the theoretical prediction  $\Sigma(\Gamma) = \Sigma(0) - 2k_B T \Gamma$  [2,4]. Here,  $C$  denotes the bulk concentration of the adhesive particles. Note that  $\Sigma = 0$  at  $\Gamma \approx 0.1/d^2$ . (Right) The adsorption layers affect the lateral stress profile  $s(z)$  in the region of the head-group layers.

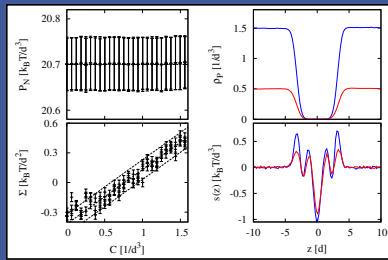


Figure 4: Symmetric depletion layers on a symmetric bilayer membrane. (Left) Membrane tension  $\Sigma$  increases with the bulk concentration  $C$  of the non-adhesive particles. The membranes have no tension at  $C \approx 0.7/d^3$ . (Right) The depletion layers affect the lateral stress profile  $s(z)$ .

## References

- [1] J.C. Shillcock and R. Lipowsky, J. Chem. Phys. 117, 5048 (2002).
- [2] B. Różycki and R. Lipowsky, J. Chem. Phys. 142, 054101 (2015).
- [3] B. Różycki and R. Lipowsky, J. Chem. Phys. 145, 074117 (2016).
- [4] R. Lipowsky, Faraday Discuss. 161, 305-331 (2013).

## Spontaneous curvature

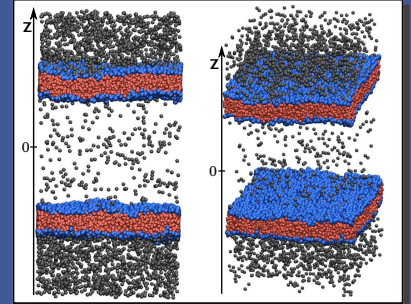


Figure 5: Two lipid bilayers exposed to adhesive particles, which do not permeate the membranes on the simulation time scales of several microseconds. Water is not shown.

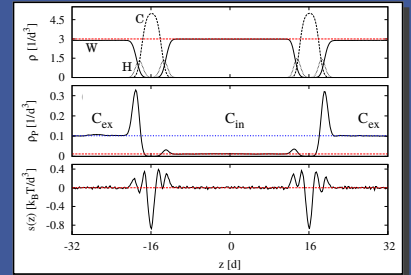


Figure 6: Density and stress profiles for two bilayer membranes shown in Fig. 5. The membranes are in a tensionless state.

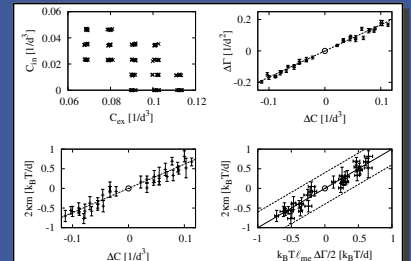


Figure 7: Results obtained from the density and stress profiles of tensionless membranes as shown in Fig. 6. Both the difference in the leaflet coverage,  $\Delta\Gamma$ , and the spontaneous curvature,  $m$ , are proportional to the bulk concentration difference  $\Delta C$ . The spontaneous curvature  $m$  is determined from the first moment of the stress profile via  $2\kappa m = \int z s(z) dz$  at the tensionless state with  $\Sigma = 0$ . Here,  $\kappa$  is the bending rigidity modulus of the membrane. The simulation results are consistent with the theoretical prediction  $4\kappa m = k_B T \ell_{me} \Delta\Gamma$  [2,4] for the effective membrane thickness  $\ell_{me} = 7.2d \approx 5.8$  nm.

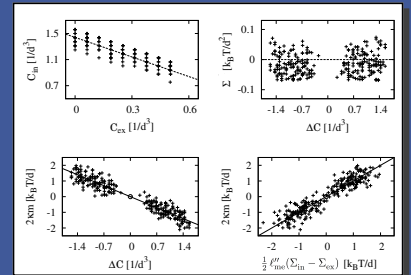


Figure 8: Analogous to Fig. 7 but for asymmetric depletion layers. The simulation data correspond to membranes in the tensionless state. The simulation results are consistent with the theoretical relation  $4\kappa m = \ell_{me}^* (\Sigma_{in} - \Sigma_{ex})$ , where  $\Sigma_{in}$  and  $\Sigma_{ex}$  denote the surface tensions of the two leaflets; the best fit to the simulation data is obtained for an effective membrane thickness  $\ell_{me}^* = 6d$ .