1251-Pos Board B143
Determining the Gaussian Curvature Modulus of Lipid Membranes in Simulations: A Comparative Study via Global Shape Transformations and Local Stress Distributions
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The Gaussian curvature modulus x-bar in silico by monitoring patch-closure processes of pre-curved circular bilayers. Applying this method to two different coarse-grained (CG) membrane models, namely the generic Cooke model [1] and the more finely-resolved and systematically parameterized MARTINI model [2], we find elastic ratios between the two curvature moduli, x-bar/k, in the range between ~0.85 and ~1.05, in line with previous estimates in literature. Yet, for the same systems studied, another well known method, which derives the material parameters from moments of the lateral stress profile, produces results that are neither in accordance with the patch-closure method nor, in fact, physically plausible. One notable observation is that the second method, which does not consider lipid-lipid correlations. Our study hence raises concerns about attempts to derive curvature-elastic properties using the stress profile method.

1252-Pos Board B144
Elasticity of Lipid Bilayer Membranes at the Nanoscale: The Need for New Terms
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Transmembrane proteins that have a hydrophobic mismatch with the membrane induce membrane thickness deformations at the nanoscale [1]. We put forward a modification to continuum elastic models describing membrane thickness deformations [2]. We show that contributions involving the gradient (and the Laplacian) of the area per lipid are significant and should be accounted for in the effective Hamiltonian per lipid from which the effective Hamiltonian of the bilayer is constructed, in the spirit of Ref. [3]. We compare the predictions of our model with numerical data giving the profile of membrane thickness close to a mismatched protein [4,5], and with experimental data on gramicidin lifetime [6] and formation rate [7].

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Opening Barrier Renormalization by Membrane Local Curve Fluctuations around the Mechanosensitive Channel: Analytical Expression
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We calculate renormalization of the opening energy barrier of mechanosensitive channel by local curvature fluctuations: U= U0 + Ua, Eq. (1), P(x,z) and P(z,h) are lateral pressure profiles in the flat and curved bilayer respectively, H and A(z) are local mean curvature and the difference between open/closed cross-section profile functions. P(x,z) is derived in [1] analytically using flexible strings model of lipid chains [2]. The average over fluctuations of the membrane’s shape h(x,y) in the Monge representation [3] uses Boltzmann factor of a curved conformation exp(-F(h)/T) with elastic free energy functional F(h) taken in the Helmholtz form, Eq. (3); k and r are bending rigidity and surface tension. Comparing our results with molecular dynamics data [4] for curved bilayers, we estimate relative importance of the contributions of the lipid tails and phospholipid headgroups to the energy barrier U. References:

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Membrane Interaction and Curvature Generation by the COPI GTPase Arf6
Sebastian Daum, Annette Meister, Kirsten Bacia
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The formation of COPI-transport vesicles and fission from the Golgi membrane proceeds via local deformation of the lipid bilayer by a curvature generating