Studying extremely large lipid membrane curvatures

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We present molecular simulation setup to study membrane curvature induced by artificial ridges. We use the coarse grain Martini force field to simulate pure DOPC and ternary mixtures lipid bilayers deposited on a solid support. For a flat scaffold, we investigate the effect of the support on basic membrane properties such as lateral diffusion and tail order parameters as a function of support properties. For the ternary mixture we additionally the effect on the degree of lateral phase separation. We find that already when the scaffold and bilayer are separated by a small water layer (>0.2 nm), the bilayer properties are unaffected. Next, we introduce a solid support with block-shaped ridges, which induce strong curvature in the lipid membrane. The effect of curvature on the bilayer properties is investigated. A dependence of the lipid order parameters on local curvature is found, as well as an overal amplifying effect on lateral phase separation.