Composition-Curvature Coupling in Binary Lipid Membranes

Marcus Müller [C, S] and Israel A. Barragan Vidal
Institute for Theoretical Physics, Georg-August University, Göttingen, Germany
mmueller@theorie.physik.uni-goettingen.de

Carla M. Rosetti
Departamento de Química Biológica, Universidad Nacional de Cordoba, Cordoba, Argentina

Claudio Pastorino
Departamento de Física de la Materia Condensada, Centro Atómico Constituyentes, CNEA/CONICET, Buenos Aires, Argentina

The coupling between local composition fluctuations in binary lipid membranes and curvature affects the lateral membrane structure. It can result in the formation of spatially modulated stripe phases and has been implicated in the formation of lipid rafts. We propose an efficient method to compute the composition-curvature coupling in molecular simulations and apply it to two coarse-grained membrane models—a minimal, implicit-solvent model and the MARTINI model. Both the weak-curvature behavior that is typical for thermal fluctuations of planar bilayer membranes as well as the strong-curvature regime corresponding to narrow cylindrical membrane tubes are studied by molecular dynamics simulation. The simulation results are analyzed by using a phenomenological model of the thermodynamics of curved, mixed bilayer membranes that accounts for the change of the monolayer area upon bending. Additionally the role of thermodynamic characteristics such as the incompatibility between the two lipid species and asymmetry of composition are investigated.