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Modeling co-evolution of defects and curvature in lipid vesicles: coarse-grained simulation studies[1] ROBIN SELINGER, JUN GENG, JONATHAN SELINGER, Kent State Univ. — To explore interaction between topological defects and curvature in lipid vesicles, we present a coarse-grained simulation approach in which defects and vesicle shape both evolve in time. First we model a vesicle cooled into the tilted gel phase. To represent the tilt field at the mesoscale, we superimpose an XY model onto a coarse-grained liquid membrane [1] where each particle represents a patch of lipid bilayer. The presence of two +1 defects drives the vesicle to a prolate equilibrium state as previously predicted; but extra +1/-1 defect pairs may induce a highly disordered shape which is deeply metastable. We discuss comparison with relevant experiments. Next we consider a lipid vesicle with nematic order, e.g. composed of lipids with a rod-shaped head group. With weak coupling between defects and curvature, the vesicle is spherical with four +1/2 defects. With stronger coupling, the vesicle becomes prolate with two defects clustered at each end. As coupling is further increased, pores nucleate at the defects and coalesce, producing a hollow cylinder. We compare simulation results with theoretical predictions and consider further applications e.g. to study tilt and defects in gel phase lipid rafts.

[1] H. Yuan et al, *Phys Rev E* 82 (2010) 011905

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