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Coarse-grained simulation of lipid vesicles with "n-atic" orientational order[1] JUN GENG, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State University, Ohio 44242, USA — We perform coarse-grained simulation studies of fluid lipid vesicles with in-plane "n-atic" orientational order associated with the shape of lipid head group, to test the theoretical predictions of Park, Lubensky and MacKintosh [1] for resulting vesicle shape and defect structures. Our simulation model uses a single layer coarse-grained implicit-solvent approach proposed by Yuan et al [2], with addition of an extra vector degree of freedom representing in-plane orientational order. We carry out simulation studies for n=1 to 6, examining in each case the spatial distribution of defects and resulting deformation of the vesicle. An initially spherical vesicle (genus zero) with n-atic order has a ground state with 2n vortices of strength 1/n, as expected, but the observed equilibrium shapes are sometimes quite different from those predicted theoretically. For the n=1 case, we find that the vesicle may become trapped in a disordered, long-lived metastable state with extra +/- defects whose pair-annihilation is inhibited by local changes in membrane curvature, and thus may never reach its predicted ground state.

[1] J. Park, T. C. Lubensky, and F. C. MacKintosh, Europhys. Lett. 20, 279 (1992)
[2] H. Yuan, C. Huang, Ju Li, G. Lykotrafitis, and S. Zhang, Phys. Rev. E 82, 011905 (2010)

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Jun Geng
Liquid Crystal Institute, Kent State University, Ohio 44242, USA

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