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Simulations of buckling of gel-phase lipid bilayers JAMES KINDT,

Emory University, Department of Chemistry — The structure of lipid bilayer vesicles below the main chain transition temperature is believed to be approximately polygonal, based on evidence of faceting from electron microscopy. The structure and mechanics of the interfaces between facets, (ridges) are issues that may be pertinent to the rate of trans-bilayer permeability as well as vesicle melting. Here we present evidence from atomistic molecular dynamics simulations that the preferred angle between facets is strongly dependent on the tilt orientation of lipid tails with respect to the ridge vector.

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